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### **TABLE OF CONTENTS**

# Volume 1 Number 1 September 2010 Sorption Characteristics of CO2 on Rocks and Minerals in Storing CO2 Processes T. Fujii, S. Nakagawa, Y. Sato, H. Inomata, T. Hashida. 1 Evaluation of Various Linear Regression Methods for Downscaling of Mean Monthly Precipitation in Arid Pichola Watershed 1 M. K. Goyal, C. S. P. Ojha. 11 Modeling of Asphaltene Grading in Oil Reservoirs 11 J. Y. Zuo, O. C. Mullins, C. L. Dong, D. Zhang. 19 Combined Generalized Hubbert-Bass Model Approach to Include Disruptions When Predicting Future Oil Production 28 Modelling Irrigation and Salinity Management Strategies in the Ord Irrigation Area 34

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# Sorption Characteristics of CO<sub>2</sub> on Rocks and Minerals in Storing CO<sub>2</sub> Processes

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### ABSTRACT

As  $CO_2$  is injected into pore spaces of water-filled reservoir rocks, it displaces much of the pore fluids. In short terms (several to tens of years), the greater part of the injected  $CO_2$  is predicted to stay as free  $CO_2$ , i.e. in a  $CO_2$  rich dense phase that may contain some water. This paper investigates the sorption characteristics for rocks (quartzose arenite, greywacke, shale, granite and serpentine) and minerals (quartz and albite) in the  $CO_2$  rich dense phase. The measurements were conducted at 50°C and 100°C, and pressures up to 20 MPa. Our results demonstrated that significant quantities of  $CO_2$  were sorbed with all the samples. Particularly, at 50°C and 100°C, quartzose arenite showed largest sorption capacity among the other samples in higher pressures (>10 MPa). Furthermore, comparison with model prediction based on the pore filling model, which assumed that  $CO_2$  acts as filling pore spaces of the rocks and minerals, suggested the importance of the sorption mechanism in the  $CO_2$  geological storage in addition to the pore-filling mechanism. The present results should be pointed out that the sorption characteristics may have significant and meaningful effect on the assessment of  $CO_2$  storage capacity in geological media.

Keywords: Sorption Characteristics, Rocks, Minerals, Storing CO<sub>2</sub> Processes, CO<sub>2</sub> Geological Storage

### **1. Introduction**

It is a well-established fact that the concentrations of CO<sub>2</sub> in the atmosphere have been increasing steadily and has increased globally by about 100 ppm (36%) over the last 250 years, from a range of 275 to 285 ppm in the pre-industrial era to 379 ppm in 2005 [1], and predictions are that, if continuing in a business-as-usual scenario, by the end of this century, humankind will be facing significant climate change, which may affect human health [2]. Thus, a major challenge in mitigating the climate change is a deep reduction of anthropogenic CO<sub>2</sub> emissions to the atmosphere, which hopefully will lead to a stabilization of CO<sub>2</sub> concentration at around 550 ppm (i.e., double of the pre-industrial level). However, the challenge of stabilizing atmospheric CO<sub>2</sub> levels becomes increasingly difficult as the problem matures because fossil fuels, which today provide about 75% of the world's energy, are likely to remain a major component of the world's energy supply for at least the next century.

In recent years, there are a number of ways by which  $CO_2$  emissions can be reduced, among them being  $CO_2$  capture and geological storage (CCGS) technology. CCGS

technology is an enabling technology that will allow the continued use well into this century of fossil fuels for power generation and combustion in industrial processes and also has the potential of the deepest cuts in anthropogenic  $CO_2$  emissions from large stationary sources (e.g., power generation, iron and steel production, cement manufacture). The technology involves the deployment of a set of technologies for capturing  $CO_2$  emitted from the large stationary sources, transporting it usually by pipeline and injecting it into geological storage reservoirs, including depleted oil and gas reservoirs, unminable coal seams, and deep saline aquifers, which is filled with water (most commonly formation brine) into pores spaces of reservoir rocks.

In terms of  $CO_2$  migration process in the deep saline aquifers, if  $CO_2$  moves into, or invades a porous medium saturated with formation brine, the latter is displaced from some of the pore space (a process referred to as drainage) [3], and then the injected  $CO_2$  stays in the injection zone for a long time, is dissolved in the formation brine, and becomes trapped by mineralization. The extent of  $CO_2$ -water-rock interaction during migration of the injected  $CO_2$  is the main control on the fate of the  $CO_2$ .

Johnson *et al.* [4] has reported that reactive transport modeling of a Sleipner-like storage reservoir, which is the world's first saline-aquifer  $CO_2$  storage site that the fate and transport of injected  $CO_2$  has been successfully monitored by seismic time-lapse surveys, suggested that 15-20% was still dissolved in the formation brine after 20 years. The remainder stayed as an immiscible condition, *i.e.* in a  $CO_2$  rich dense phase that may contain little water. Consequently, the result from this study indicates that, through the  $CO_2$  migration process within the deep saline aquifers, the fate of injected  $CO_2$  would be predicted to be mostly the immiscible condition in the order of short term storage (e.g. several years or ten years).

Many researchers have investigated about mineral trapping processes among  $CO_2$ , water, and rock in  $CO_2$ -water-rock system [5-9]. However, interactions among  $CO_2$  and rock that simulates the  $CO_2$  rich dense phase have only been conducted by Lin *et al.* [10].

Up to now, gas sorption isotherm experiments in CO2/rock or CO2/water/rock systems have been conducted using shale at 45-50°C and pressures up to 20 MPa [11] and sandstone and granite at 33-200°C, and pressures up to 20 MPa [12-14]. Fujii et al. [13,14] indicates that at high pressures (> 10MPa), the amount of  $CO_2$  sorbed by granite is comparable to that by sandstone, but the sorption mechanisms and processes for sandstone, shale, and granite has not been elucidated. Therefore, knowledge of CO<sub>2</sub> sorption characteristics for various rocks will be required for the screening and assessment of suitable  $CO_2$  storage sites for sequestration of  $CO_2$  in geological reservoirs. Thus, for this comparison, in addition to the rock samples reported in the previous literatures, we included samples from other types of rocks (e.g., sedimentary rock, volcanic rock, metamorphic rock) in this experiment. Additionally, to better understand the mechanisms related to sorption of CO2 on rocks, CO2 sorption measurements for silica and silicate minerals, which are main component of reservoir rocks, were also conducted.

The purpose of this study is to evaluate sorption characteristics of  $CO_2$  for rocks (sedimentary rocks, metamorphic rocks, and volcanic rocks) and minerals (silica and silicate minerals) in the  $CO_2$  rich dense phase at geological-relevant temperatures and pressures.

### 2. Experimental

### 2.1. Samples and Preparation

Samples from five different blocks of rocks (quartzose arenite, greywacke, shale, granite, and serpentine) were used in the experiments. Quartzose arenite and grey-

wacke are well known as quartz-rich sandstone and feldspar-rich sandstone, respectively. In this study, Berea sandstone (from Ohio, USA) and Kimachi sandstone (from Shishido-cho, Shimane, Japan) were chosen as the representation of quartzose arenite and greywacke, respectively.

Berea sandstone composition was determined by point counting (500 points) under a polarizing microscope (OLYMPUS, A6400BX). Berea sandstone consisted mainly of quartz (= 90.7 vol. %), and the observation was in agreement with the results of Wang and Nur (1989). Kimachi sandstone consisted mainly of plagioclase (= 89.9 vol. %) [15]. A sample of shale was obtained from Tedori-group, Niigata, Japan. A sample of granite was obtained from Iidate, Fukushima, Japan. The granite consisted mainly of quartz (= 37.1 vol. %), plagioclase (= 34.0 vol. %) and K-feldspar (= 21.8 vol. %) [15]. A sample of serpentine was obtained from Okaya, Nagano, Japan. Examination of the serpentine using X-ray diffraction verified the abundance of chrysotile and lizardite. Additionally, natural single crystals of quartz (from Alto de Cruzes Santander, Colombia) and albite (from Kotaki, Itoigawa, Niigata, Japan) were used in the experiment. These rock and mineral specimens were shown in Figure 1.

The American Society for Testing and Materials (ASTM) procedure [16] was used to determine density and porosity of the samples based on the fundamental Archimedes principle. Specific surface areas were determined by low-pressure nitrogen sorption measurements using the Brunauer-Emmett-Teller (BET) method [17]. The nitrogen sorption measurements were performed at 77 K using a Quantachrome NOVA 2000 series automated volumetric instrument. Prior to each analysis, the samples were degassed at 105°C under vacuum. The obtained values were listed in **Table 1**.

Core specimens of Berea sandstone, Kimachi sandstone, and Iidate granite were cored from these blocks with a thin-wall diamond bits and were cut with a diamond saw. All cores were drilled perpendicular to the bedding plane. These core specimens were each about 16 mm in diameter and about 10 mm in length. The specimen of shale was broken into angular fragments approximately 5 to 10 mm in largest dimension. The specimen of serpentine was cut into approximately  $10 \times 10$ mm<sup>2</sup> in cross-section and 15 mm in length. The specimens of quartz and albite with dimensions of  $65 \times 20$ mm<sup>3</sup> and  $10 \times 10 \times 10$  mm<sup>3</sup>, respectively, were prepared from each natural single crystals.

These cut specimens were washed with distilled water and were dried under vacuum in an oven for at least 24 hours at 105°C using a rotary vacuum pump.





(e)



<u>5 mm</u>

(d)

Figure 1. Photographs of rock and mineral specimens tested in the experiment. (a) Berea sandstone; (b) Kimachi sandstone; (c) Shale; (d) Serpentine; (e) Granite; (f) Quartz; (g) Albite.

Materials	Specific surface area (m <sup>2</sup> /g)	Bulk density (g/cm <sup>3</sup> )	Porosity (vol. %)
Kimachi sandstone	2.80	2.51	20.0
Berea sandstone	0.84	2.11	19.0
Granite	-	2.62	1.1
Shale	0.65	2.60	3.4
Serpentine	-	2.51	4.9
Quartz	-	2.60	< 0.1
Albite	-	2.60	0.9

Table 1. Rocks and minerals properties for CO<sub>2</sub> sorption measurement.

### 2.2. Apparatus and Procedure

The magnetic suspension balance (MSB) from Rubotherm Präzisionsmesstechnik GmbH [18] rated at 350°C and 35 MPa was used to measure the CO<sub>2</sub> sorption capacity of rocks and minerals, as illustrated in **Figure 2**. The MSB consisted of a sorption chamber that was used to expose the sample to CO<sub>2</sub> at elevated temperatures and pressures, and microbalance, which was isolated from the sample and existed at ambient conditions. All of the details for the MSB and its operational procedures have been described in previous literatures by Sato *et al.* [19] and Blasig *et al.* [20]. A schematic of the experimental apparatus was shown in **Figure 3**. The experimental apparatus consisted of a high CO<sub>2</sub> pressure supply system, which was used to pressurize CO<sub>2</sub> up to 20 MPa, a data acquisition system and a MSB system.

In the experiment, the sorption measurements were performed at  $50^{\circ}$ C and  $100^{\circ}$ C, and pressures up to 20 MPa.

In a typical experiment, a sample was weighed and placed in a sample basket suspended by a permanent magnet through an electromagnet, as shown in **Figure 2**. After closing the sorption chamber, the sample was degassed by evacuating the sorption chamber at elevated temperatures until the weight measured by the microbalance remained unchanged over time. A heating circulator (Julabo, model F25) was used to control the temperature of the chamber, which was measured with a calibrated platinum resistance thermometer to an accuracy of  $\pm 0.05$ 



Figure 2. Principle of the magnetic suspension balance (MSB).



Figure 3. Schematic diagram of the experimental apparatus for CO<sub>2</sub> sorption measurement by using the MSB system (source: Sato *et al.* [19]).

K. The sample weight, read from the microbalance under vacuum and at temperature *T*, was recorded as w (*vac*, *T*) prior to CO<sub>2</sub> injection into the sorption chamber.

 $CO_2$  was introduced into the sorption chamber by the following way. At low pressure up to 5 MPa, the sorption chamber was flooded with  $CO_2$  from a gas cylinder and the pressure was controlled by a regulator. Whereas, at the pressures above 5 MPa,  $CO_2$  was introduced by passing through a high-performance liquid chromatography (HPLC) pump (Jasco 880PU).  $CO_2$  pressure inside the sorption chamber was measured by using Paroscientific pressure transducer (46KR, 41.4 MPa F.S., accuracy 0.01% F.S.).

The change in the mass of the sample as well as the temperature and pressure were measured continuously until the thermodynamic equilibrium was reached. Eventually, an equilibrium sorption was reached, that is, the mass of the sample stopped increasing. The equilibrium sorption was achieved in about 90 minutes at every pressure steps. At this final saturation stage, the weight reading from the microbalance at pressure P and temperature T was recorded as w(P, T).

The mass of the sorbed  $CO_2$  on the rock and mineral samples was calculated based on the consideration of a buoyancy of instruments, which was housed in the sorption chamber, at different gas pressures and different densities as shown in the Equation (1).

Where  $n_g^{ex}(P, T)$  was CO<sub>2</sub> sorbed amount on the sample and was termed excess CO<sub>2</sub> sorption capacity.  $\rho_{CO2}(P, T)$ was CO<sub>2</sub> phase density at *P* and *T*.  $m_{CO2}$  was the molecular weight.  $V_r$  and  $V_b$  were the volumes of the sample and of the sample basket, respectively. The last term of the above equation,  $\rho_{CO2}(P, T) \cdot (V_b + V_r)$  represented the buoyancy force caused by the compressed gas, which lifted the sample and sample basket. CO<sub>2</sub> phase density,  $\rho_{CO2}(P, T)$ , was calculated from the Wagner EOS [21].

The volume of the sample basket,  $V_b$ , was determined using Equation (2) from a buoyancy experiment, that is, the MSB experiment was performed without a sample in the sample basket at the experimental temperature and pressure.

$$V_{b} = \left\{ w(vac, T) - w(P, T) \right\} / \rho_{CO_{2}}(P, T)$$
(2)

The result obtained from the buoyancy experiment indicated that, at 50°C and 100°C, the values of the sample basket were constant within limited pressure ranges (~20 MPa) and were 1.69 cm<sup>3</sup> at 50 °C and 1.71 cm<sup>3</sup> at 100°C, respectively. The volume of the sample,  $V_r$ , was calculated from mass and density of the sample. After the experiment, the samples were reweighed under vacuum condition in the sorption chamber.

### 3. Results and Discussion

The excess sorption data of  $CO_2$  obtained on the five rock samples (Berea sandstone, Kimachi sandstone, serpentine, shale, granite) and the two mineral samples (quartz and albite) are shown in **Figure 4** under the pressures up to 20 MPa at 50°C in **Figure 4(a)** and 100°C in **Figure 4(b)**, respectively.

The excess sorption data are shown on a sample volume basis in Figure 4. It has been shown that shale [11] and sandstone and granite [12-14] have a certain degree of sorption capacities for CO<sub>2</sub> under air-dry conditions. The experimental data obtained in this study confirm the results of the previous literatures. Figure 4 reveals that the Berea sandstone samples show significantly larger weight changes compared with the other types of rocks, in particular with the Kimachi sandstone samples. The maximum sorption capacity of Berea sandstone for CO<sub>2</sub> exhibits 3.7 mmol/cm<sup>3</sup> (=  $82.9 \text{ cm}^3 \text{ STP/cm}^3$ ) at 50°C and 20 MPa and 2.8 mmol/cm<sup>3</sup> (=  $62.7 \text{ cm}^3 \text{ STP/cm}^3$ ) at 100°C and 20 MPa, respectively. It should be mentioned here that the pore volume of Berea sandstone (porosity:  $\phi$  17.9 vol.%) is slightly smaller than that of Kimachi sandstone (porosity:  $\phi 20.0$  vol. %). As mentioned in the section of Experimental, B.E.T. tests were carried out to evaluate the specific surface area of the rock samples using N<sub>2</sub> sorption isotherms. Valid experimental data for specific surface area were obtained only for Berea sandstone, Kimachi sandstone, and shale, which showed no dependence of the sample sizes used for the B.E.T. tests. In contrast, the other types of rocks exhibited specific surface areas which varied with the sample size used. In view of the B.E.T. results, the excess sorption data per unit surface area are given only for Berea sandstone, Kimachi sandstone, and shale in Figures 5(a) and 5(b). It is apparent that Berea sandstone outperforms Kimachi sandstone and shale in the CO<sub>2</sub> sorption capacity.

Coal studies on sorption revealed that maximum excess  $CO_2$  sorption values were approximately 2.0 mmol/g for various coal samples on dry basis at around 50°C [22-24]. Based on  $CO_2$  gravimetric capacity for the rock and mineral samples, at 50°C, maximum  $CO_2$  excess sorption values were approximately 1.8 and 0.5 mmol/g for Berea sandstone and the other rock and mineral samples, respectively. It can, therefore, be said that Berea sandstone exhibits comparable capacity as coals and has a significantly sorption capacity.

$$n_{g}^{ex}(P,T) = \left\{ w(P,T) - w(vac,T) + \rho_{CO_{2}}(P,T) \cdot (V_{b} + V_{r}) \right\} / m_{CO_{2}}$$

$$\tag{1}$$

Excess Sorption (mmol/cm<sup>3</sup>) 4.0 ndetona Excess Sorption (mmol/cm<sup>3</sup>) 4.0 Berea sandstone Kimachi sandston Kimachi sandston 3.5 3.5 Shale Shale Serpentine Serpentin 3.0 3.0 Granite Granite Albite Albite 2.5 2.5 Quartz Quartz 2.0 2.0 1.5 1.5 1.0 1.0 0.5 0.5 0.0 0.0 0 5 10 15 20 0 5 10 15 20 Pressure (MPa) Pressure (MPa) (b) (a)

Figure 4. Gravimetric  $CO_2$  excess sorption uptake per unit volume for rocks and minerals under air-dry condition in  $CO_2$ /rock or  $CO_2$ /mineral systems: (a) at 50°C and (b) at 100°C.



Figure 5. Gravimetric  $CO_2$  excess sorption uptake per unit surface area for rocks and minerals under air-dry condition in  $CO_2$ /rock or  $CO_2$ /mineral systems: (a) at 50°C and (b) at 100°C.

It is also shown in **Figure 4** that the two mineral samples (quartz and albite) are capable of sorbing  $CO_2$  in the  $CO_2$  rich dense phase. Both quartz and albite is a common and fundamental constitutes of most types of rocks. The above result for the quartz and albite samples suggests that the  $CO_2$  sorption capacity of the rocks tested in this study can be attributed to the sorption of  $CO_2$  onto silica and silicate minerals.

It is shown in **Figure 4(a)** that the sorption isotherms at 50°C exhibit a rapid increase in the excess  $CO_2$  sorption for more or less all the rocks and minerals tested, even though the increasing trend is unclear except for Berea sandstone. The rapid increase in the excess  $CO_2$ sorption takes place when the pressure exceeds the critical point of  $CO_2$  (31.0°C, 7.38 MPa) for 50°C. In contrast, the results for 100 °C show a nearly linear increase trend with increasing pressure for the majority of the rocks and minerals. It is interesting to note that the results may correlate with the pressure dependence of  $CO_2$  density. In fact, the  $CO_2$  density shows a sharp jump at the critical point of  $CO_2$  for 50°C, whereas an approximately linear increase is observed for 100°C [21].

The amount of CO<sub>2</sub> sorbed at 50°C decreases with increasing pressure in the higher pressure range (> 10 MPa), except for Berea sandstone. This trend is in agreement with the result reported by Romanov *et al.* [22], who have shown for coal samples that at high pressures above 10 MPa, the amount of CO<sub>2</sub> sorbed reduced as increasing pressure.

The decreasing trend of the sorption isotherms for  $50^{\circ}$ C in the high pressures may be due to the buoyancy force acting on the volume of sorbed CO<sub>2</sub> phase. The sorbed CO<sub>2</sub> phase may alter the buoyancy of the sample in the ambient CO<sub>2</sub> pressures and temperatures during

the experiment, in addition to the volume of the sample,  $V_{\rm r}$ , the sample basket,  $V_{\rm b}$ , and the other measurement instrument. However, the calculation of the excess CO<sub>2</sub> sorption capacity based on Equation (1) ignores the buoyancy effect of the volume of the sorbed CO<sub>2</sub> phase, thus introducing error. Therefore, the error caused by the above-mentioned buoyancy force would be larger at the high pressure range (above the critical pressure) than the low pressure region (~5 MPa) because the CO<sub>2</sub> density and the sorbed phase volume usually increases as the CO<sub>2</sub> pressure increases. The observation suggests that the buoyancy effect may cause the reduction in the excess sorption for the high pressure range.

The amount of sorbed  $CO_2$  for Berea sandstone, however, showed a monotonous increase with increasing  $CO_2$ pressure, even in the higher pressure range. The comparison suggests that the sorption mechanism may form a denser  $CO_2$  sorbed phase in the case of Berea sandstone. The reason for this is unclear and requires further investigation.

As shown in **Figure 4(b)**, the sorption capacity for  $100^{\circ}$ C is lower compared with the results for  $50^{\circ}$ C and shows an approximately linear increase up to 20 MPa, except for Kimachi sandstone.

In contrast, no decreasing trend in the excess sorption is observed for 100°C. Reason for this may be attributed to the decrease of the buoyancy force due to the temperature increase. The buoyancy force associated with sorbed phase volumes was mainly determined by the density of CO<sub>2</sub> phase and CO<sub>2</sub> sorbed phase, and the CO<sub>2</sub> sorption amount. The value of CO<sub>2</sub> density calculated by the Span and Wagner EOS [21] for 100°C and 20 MPa is shown to be approximately half as much as that at 50°C. In addition, the sorbed phase density predicted by Dubinin (1965) [25] decreases with increasing temperature. These results indicates that the buoyancy effect for 100°C is smaller that than for 50°C. Consequently, the error induced by the buoyancy effect for 100°C may be smaller than that for 50°C.

Sorption and desorption isotherms are shown for Berea sandstone and serpentine at 50°C in **Figure 6**. The desorption isotherms coincide approximately with the sorption data. Furthermore, weight measurements for the samples have shown almost no change after the  $CO_2$  sorption experiment. These results indicate the reversible nature of  $CO_2$  sorption-desorption process at 50°C. The same trend has been observed for 100°C.

### 4. Comparison with Prediction Value Based on Pore-Filling Model

Based on the above discussion, the experimental excess sorption data are corrected for the buoyancy force for the sorbed phase volume using the following equation [26]:



Figure 6. Excess sorption and desorption isotherms of  $CO_2$  at 50°C for (a) Berea sandstone and (b) Serpentine under air dry condition in CO2/rock system.

$$n_{g}^{c} = n_{g}^{ex} \cdot \left(\frac{\rho_{a}}{\rho_{a} - \rho_{CO_{2}}\left(P,T\right)}\right)$$
(3)

where  $n_g^c$  is the CO<sub>2</sub> sorption capacity corrected for the buoyancy effect,  $n_g^{ex}$  is the sorbed amount without correction (as measured by the MSB method),  $\rho_{CO2}(P,T)$  is the CO<sub>2</sub> density of the gas phase, and  $\rho_a$  is the CO<sub>2</sub> density of the sorbed phase. In this study, we used the sorbed phase density,  $\rho_a$ , calculated by Dubinin-Nikolaev formulation [25]. The value of  $\rho_a$  is usually assumed to be constant over the entire pressure range at temperatures above the critical temperature (31.1°C). The calculated values of  $\rho_a$  at 50 °C and 100 °C were 0.994 g/cm<sup>3</sup> and 0.912 g/cm<sup>3</sup>, respectively. The CO<sub>2</sub> phase density,  $\rho_{CO2}$ (*P*, *T*), was calculated from Span and Wagner EOS [21]. The data for the corrected sorption amount are shown in **Figures 7** and **8**. In addition to the corrected CO<sub>2</sub> sorption



Figure 7. Comparison of the predicted values based on the pore-filling model, with corrected sorption capacity, considering CO<sub>2</sub> sorbed phase density for three sedimentary rocks (Berea sandstone, Kimachi sandstone, and shale), one ultramafic rock (serpentine) and one volcanic rock (granite) at 50°C and 100°C. The solid and dashed lines represent the corrected experimental data and the calculated data, respectively. () is the porosity of rock specimens. (a) Berea sandstone ( $\phi$  19.0); (b) Kimachi sandstone ( $\phi$  20.0); (c) Serpentine ( $\phi$  4.9); (d) Shale ( $\phi$  3.4); (e) Granite ( $\phi$  1.1).

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Figure 8. Comparison of the predicted values based on the pore-filling model, with corrected sorption capacity, considering  $CO_2$  sorbed phase density for quartz and albite at 50°C and 100°C. The solid and dashed lines represent the corrected experimental data and the calculated data, respectively. () is the porosity of mineral specimens. (a) Quartz ( $\phi 0.1$ ); (b) Albite ( $\phi 0.9$ ).

data, the results predicted from the pore-filling model are plotted in these figures. The pore-filling model assumes that the  $CO_2$  storage capacity of the rock mass is equal to the amount of  $CO_2$  used to fill the pore volume in the rock, which is given by the following equation:

$$n_{pore-filling} = \phi_{rock} \cdot \rho_{CO_2} / m_{CO_2}$$
(4)

where  $\phi_{\text{rock}}$  is the porosity of the rock sample, and  $m_{\text{CO2}}$ is the molecular weight of CO<sub>2</sub>. It is seen that the sorption capacity corrected for the buoyancy effect shows a steady increase with respect to pressure at the higher pressure regime, except for the data of the granite and albite at 50°C. The reason for this result probably may be due to the error in estimating the sorbed phase density, and needs to be further investigated in the future. In the lower pressure range (< 5 MPa), the corrected sorption capacity appears to give a value close to that computed based on the pore-filling model. It is demonstrated that the corrected sorption capacity is significantly higher than the model predicted data for the rocks and minerals, except for Kimachi sandstone. For Kimachi sandstone, the corrected result is relatively close to the model predicted data over the entire pressure range. For example, the corrected sorption capacity is shown to be approximately 5 times higher than the model prediction in the case of Berea sandstone, and about 10 times higher for the granite. The comparison may suggest the importance of the sorption mechanism in the  $CO_2$  geological storage in addition to the pore-filling mechanism. The sorption process may provide an additional CO<sub>2</sub> storage mechanism and contribute to the significant part of the CO<sub>2</sub> storage capacity of a rock mass. The effect of water and salinity on the CO<sub>2</sub> sorption capacity is now under investigation.

### 5. Conclusions

This paper presents the  $CO_2$  sorption capacities of the five rock samples (Berea sandstone, Kimachi sandstone, shale, serpentine and granite) and the two mineral samples (quartz and albite), measured at 50°C and 100°C, and under pressures up to 20 MPa in CO<sub>2</sub>-rock or CO<sub>2</sub>-mineral systems that simulate the CO<sub>2</sub> rich dense phase. The CO<sub>2</sub> sorption capacities have been determined by a gravimetric method and corrected for the buoyancy effect. In higher pressure region (> 10 MPa), Berea sandstone has shown a significantly higher CO<sub>2</sub> sorption capacity compared to the other rocks and minerals at both 50°C and 100°C and exhibited a maximum sorption capacity of 3.7 mmol/cm<sup>3</sup> (=  $82.9 \text{ cm}^3 \text{ STP/cm}^3$ ) at 50 °C and 20 MPa and 2.8 mmol/cm<sup>3</sup> (=  $62.7 \text{ cm}^3 \text{ STP/cm}^3$ ) at 100°C and 20 MPa. Thus, arkosic sandstone such as Berea sandstone may provide a significant potential for CO<sub>2</sub> geological sequestration for a suitable reservoir rock. It is also shown that the major constituent minerals for the rocks tested in this study (quartz and albite) have a CO<sub>2</sub> sorption behavior.

It has been demonstrated that the  $CO_2$  sorption capacity measured in this study is significantly higher than that predicted by the pore-filling model for the rocks and minerals. The comparison suggests that the  $CO_2$  sorption characteristic may provide an important mechanism in the assessment of  $CO_2$  storage capacity in geological media.

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# **Evaluation of Various Linear Regression Methods for Downscaling of Mean Monthly Precipitation in Arid Pichola Watershed**

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### ABSTRACT

In this paper, downscaling models are developed using various linear regression approaches namely direct, forward, backward and stepwise regression for downscaling of GCM output to predict mean monthly precipitation under IPCC SRES scenarios to watershed-basin scale in an arid region in India. The effectiveness of these regression approaches is evaluated through application to downscale the predictand for the Pichola lake region in Rajasthan state in India, which is considered to be a climatically sensitive region. The predictor variables are extracted from (1) the National Centers for Environmental Prediction (NCEP) reanalysis dataset for the period 1948–2000, and (2) the simulations from the third-generation Canadian Coupled Global Climate Model (CGCM3) for emission scenarios A1B, A2, B1 and COMMIT for the period 2001–2100. The selection of important predictor variables becomes a crucial issue for developing downscaling models since reanalysis data are based on wide range of meteorological measurements and observations. Direct regression was found to yield better performance among all other regression techniques explored in the present study. The results of downscaling models using both approaches show that precipitation is likely to increase in future for A1B, A2 and B1 scenarios, whereas no trend is discerned with the COMMIT.

Keywords: Backward, Forward, Precipitation, Regression, Stepwise

### 1. Introduction

Global circulation models (GCMs) are important tool in assessment of climate change. These are numerical models that have been designed to simulate the past, present, and future climate [1]. These models remain relatively coarse in resolution and are unable to resolve significant subgrid scale features. In most climate change impact studies, such as hydrological impacts of climate change, impact models are usually required to simulate sub-grid scale phenomenon and therefore require input data at similar sub-grid scale. The methods used to convert GCM outputs into local meteorological variables required for reliable hydrological modeling are usually referred to as "downscaling" techniques [2,3]. Precipitation is an important parameter for climate change impact studies. A proper assessment of probable future precipitation and its variability is to be made for various water resources planning and hydro-climatology scenarios.

A number of papers have previously reviewed down-

scaling concepts, including 1) low-frequency rainfall events [4] 2) daily precipitation [5] 3)seasonal precipitation [6] 4) daily and monthly precipitation [7] 5) monthly precipitation [8] 6) monthly precipitation [9] 7) monthly precipitation [10] 8) monthly precipitation [11] 9) annual precipitation [3].

In this paper, we explore four linear regression approaches; namely, (a) direct regression, (b) forward regression, (c) backward regression and (d) stepwise regression as a downscaling methodology to study climate change impact over Pichola lake basin in an arid region. Apparently, in the literature, there appears no evidence of any study dealing with simultaneous evaluation of various regression approaches. In the light of this, the objective of this study is to 1) to rank various regression approaches 2) to downscale mean monthly precipitation using best available regression approach from simulations of CGCM3 for latest IPCC scenarios. The scenarios which are studied in this paper are relevant to Intergovernmental Panel on Climate Change's (IPCC's) fourth

assessment report (AR4) which was released in 2007.

### 2. Study Region

The area of the this study is the Pichola lake catchment in Rajasthan in India that is situated from  $72.5^{\circ}E$  to  $77.5^{\circ}E$  and  $22.5^{\circ}N$  to  $27.5^{\circ}N$ . It receives an average annual precipitation of 597 mm. It has a tropical monsoon climate where most of the precipitation is confined to a few months of the monsoon season. The south–west (summer) monsoon has warm winds blowing from the Indian Ocean causing copious amount of precipitation during June–September months.

The Pichola watershed, located in Udaipur district, Rajasthan is one of the major sources for water supply for this arid region. During the past several decades, the streamflow regime in the catchment has changed considerably, which resulted in water scarcity, low agriculture yield and degradation of the ecosystem in the study area [12]. Regions with arid and semi-arid climates could be sensitive even to insignificant changes in climatic characteristics [13]. Temperature affects the evapotranspiration [14], evaporation and desertification processes and is also considered as an indicator of environmental degradation and climate change. Understanding the relationships among the hydrologic regime, climate factors, and anthropogenic effects is important for the sustainable management of water resources in the entire catchment hence this study area was chosen because of aforementioned reasons. The location map of the study region is

### shown in Figure 1.

### 3. Data Extraction

The monthly mean atmospheric variables were derived from the National Center for Environmental Prediction (NCEP/NCAR) (hereafter called NCEP) reanalysis data set [15] for a period of January 1948 to December 2000. The data have a horizontal resolution of 2.5° latitude X longitude and seventeen constant pressure levels in vertical. The atmospheric variables are extracted for nine grid points whose latitude ranges from 22.5 to 27.5 °N, and longitude ranges from 72.5 to 77.5 °E at a spatial resolution of 2.5°. The precipitation are used at monthly time scale from records available for Pichola Lake which is located in Udaipur at 24° 34'N latitude and 73°40'E longitude. The data is available for the period January 1990 to December 2000 [12]. The Canadian Center for Climate Modeling and Analysis (CCCma) provides GCM data for a number of surface and atmospheric variables for the CGCM3 T47 version which has a horizontal resolution of roughly 3.75° latitude by 3.75° longitude and a vertical resolution of 31 levels. The data comprise of present-day (20C3M) and future simulations forced by four emission scenarios, namely A1B, A2, B1 and COMMIT. The nine grid points surrounding the study region are selected as the spatial domain of the predictors to adequately cover the various circulation domains of the predictors considered in this study. The GCM data is re-gridded to a common 2.5° using inverse



Figure 1. Location map of the study region in Rajasthan State of India with NCEP grid.

square interpolation technique [16]. The utility of this interpolation algorithm was examined in previous down-scaling studies [17,18].

### 4. Regression Approaches

In statistical methods, the order in which the predictor variables are entered into (or taken out of) the model is determined according to the strength of their correlation with the criterion variable.

In direct regression, all available predictor variables are put into the equation at once and they are assessed on the basis of proportion of variances in the criterion variable (Y) they uniquely account for.

In Forward selection, the variables are entered into the model one at a time in an order determined by the strength of their correlation with the criterion variable. The effect of adding each is assessed as it is entered, and variables that do not significantly add to the success of the model are excluded [19].

In Backward selection, all the predictor variables are entered into the model. The weakest predictor variable is then removed and the regression re-calculated. If this significantly weakens the model then the predictor variable is re-entered–otherwise it is deleted. This procedure is then repeated until only useful predictor variables remain in the model [20,21].

Stepwise is the most sophisticated of these statistical methods. Each variable is entered in sequence and its value assessed. If adding the variable contributes to the model then it is retained, but all other variables in the model are then re-tested to see if they are still contributing to the success of the model. If they no longer contribute significantly they are removed. Thus, this method should ensure that one end up with the smallest possible set of predictor variables included in one's model [22].

### 5. Selections of Predictors

For downscaling predictand, the selection of appropriate predictors is one of the most important steps in a downscaling exercise. Various authors have used large-scale atmospheric variables, namely air temperature (at 925, 500 and 200mb pressure levels), geopotential height (at 500 and 200mb pressure levels), zonal (u) and meridional (v) wind velocities (at 925 and 200mb pressure levels), as the predictors for downscaling GCM output to mean monthly precipitation over a catchment [8,10,23].

Predictors have to be selected based both on their relevance to the downscaled predictands and their ability to be accurately represented by the GCMs. Cross-correlations are in use to select predictors to understand the presence of nonlinearity/linearity trend in dependence structure [23,24]. These cross-correlations between each of the predictor variables in NCEP and GCM datasets are useful to verify if the predictor variables are realistically simulated by the GCM. Cross-correlations are computed between the predictor variables in NCEP and GCM datasets (Table 1). The cross correlations are estimated using three measures of dependence namely, product moment correlation, Spearman's rank correlation and Kendall's tau Scatter plots and cross-correlations between each of the predictor variables in NCEP and GCM datasets are useful to verify if the predictor variables are realistically simulated by the GCM. Cross-correlations between each of the predictor variables in NCEP and GCM datasets are useful to verify if the predictor variables are realistically simulated by the GCM.

### 6. Development of Downscaling Models

For downscaling precipitation, the probable predictor variables that have been selected to develop the models are considered at each of the nine grid points surrounding and within the study region. In this study, various linear regression approaches are used to downscale mean monthly precipitation in this study. The data of potential predictors is first standardized. Standardization is widely used prior to statistical downscaling to reduce bias (if any) in the mean and the variance of GCM predictors with respect to that of NCEP-reanalysis data [24]. Standardization is done for a baseline period of 1948 to 2000 because it is of sufficient duration to establish a reliable climatology, yet not too long, nor too contemporary to include a strong global change signal [24].

A feature vector (standardized predictor) is formed for each month of the record using the data of standardized NCEP predictor variables. The feature vector is the input to the linear regression models, and the contemporaneous

Table 1. Cross-correlation computed between probable predictors in NCEP and GCM datasets.

	Ta925	Ua925	Va925	Va200	Ta20	Zg200	Ua200	Ta500	Zg500
Р	0.83	0.79	0.67	-0.18	0.66	0.81	0.23	0.81	0.60
S	0.68	0.56	0.43	-0.14	0.46	0.64	0.57	0.64	0.39
K	0.87	0.76	0.61	-0.20	0.68	0.85	0.73	0.85	0.59

Here P, S and K represent product moment correlation, Spearman's rank correlation and Kendall's tau respectively.

value of predictand is the output. To develop downscaling models, the feature vectors which are prepared from NCEP record are partitioned into a training set and a validation set. Feature vectors in the training set are used for calibrating the model, and those in the validation set are used for validation. The 11-year mean monthly observed precipitation data series were broken up into a calibration period and a validation period. Four models M1, M2, M3 and M4 were developed corresponding to regression approaches namely stepwise, forward, backward and direct respectively for predictand (Precipitation). The models were calibrated on the calibration period 1990 to 1995 and validation involved period 1996 to 2000. The various error criteria are used as an index to assess the performance of the model. Based on the latest IPCC scenario, models for mean monthly precipitation were evaluated based on the accuracy of the predictions for validation data set.

### 7. Results and Discussions

Downscaling models were developed following the methodology as discussed in preceding section. The results and discussion are presented in this section.

### 7.1. Potential Predictor Selection

The most relevant probable predictor variables necessary for developing the downscaling models are identified by using the three measures of dependence following the procedure. The cross-correlations enable verifying the reliability of the simulations of the predictor variables by the GCM, are shown in **Table 1**. In general, the most of predictor variables are realistically simulated by the GCM. It is noted that air temperature at 925mb (Ta 925) is the most realistically simulated variable with a CC greater than 0.8, while meridional wind at 200mb (Va200) is the least correlated variable between NCEP and GCM datasets (CC = -0.17). It is clear from **Table 1** that air temperature at 925mb (Ta 925), air temperature at 500 mb (Ta500), air temperature at 200 mb (Ta200), meridional wind at 925mb (Va 925), zonal wind at 925mb (Ua925), zeo-potential height at 200mb (Zg200) and zeo-potential height at 500mb (Zg500) are better correlated than meridional wind at 200mb (Va200).

# 7.2. Downscaling and performance of GCM Models

Seven predictor variables namely air temperature at 925 mb, 500 mb and 200 mb, zonal wind (925 mb); meridoinal wind (925 mb); zeo-potential height 500 mb and 200 mb at 9 NCEP grid points with a dimensionality of 63, are used as the standardized data of potential predictors. These feature vectors are provided as input to the various regressions downscaling model. Results of the different regression models (viz. M1 to M4) as discussed in previous section are tabulated in **Table 2**. Some of the precipitation values using this technique resulted in negative precipitation. However, this is physically not possible to have negative precipitation on a basin. Hence, these negative values are considered zero to compute various errors.

For predictand precipitation, coefficient of correlation

Model -	C	CC	SS	SE	Μ	SE	RN	ISE
Widdei	Training	Validation	Training	Validation	Training	Validation	Training	Validation
M1	0.90	0.79	111573.52	125884.77	1549.63	2098.08	39.37	45.80
M2	0.91	0.79	111304.52	125884.77	1545.90	2098.08	39.32	45.80
M3	0.94	0.65	73875.77	182400.92	1026.05	3040.02	32.03	55.14
M4	0.95	0.60	55529.22	204162.48	771.24	3402.71	27.77	58.33
	NMSE		N-S I	Index	Μ	AE		
	Training	Validation	Training	Validation	Training	Validation		
	0.19	0.46	0.81	0.53	0.63	0.37		
	0.19	0.46	0.81	0.53	0.63	0.37		
	0.13	0.67	0.87	0.32	0.70	0.25		
	0.09	0.75	0.90	0.24	0.72	0.23		

Table 2. Various performance statistics of model using various regression approaches.

Here CC, SSE, SSE, MSE, RMSE, NMSE, N-S Index, MAE indicate Coefficient of Correlation, Standard Error of Estimate, Mean Square Error, Root Mean Square Error, Normalized Mean square Error, Nash–Sutcliffe Efficiency Index and Mean Absolute Error respectively.

(CC) was in the range of 0.65-0.95, RMSE was in the range of 27.77-58.33, N-S Index was in the range of 0.24-0.90 and MAE was in the range of 0.23-0.72 for regression based models (viz. *M*1 to *M*4) for training and validation set. It can be observed from **Table 2** that the performance of direct regression models for mean monthly precipitation are clearly superior to that of forward, backward and stepwise regression based models in training data set while the performance of stepwise and forward regression models for predictand are clearly superior to that of backward and direct regression based models in validation data set. Results of forward and stepwise regression are quite similar. It can be inferred that model *M*4 using direct regression performed best for predictand precipitation.

A comparison of mean monthly observed precipitation with precipitation simulated using forward regression models *M*4 has been shown from **Figure 2** for calibration and validation period. Calibration period is from 1990 to 1995, and the rest is validation period.

Once the downscaling models have been calibrated and validated, the next step is to use these models to downscale the control scenario simulated by the GCM. The GCM simulations are run through the calibrated and validated direct regression model *M*4 to obtain future simulations of predictand. The predictand patterns are analyzed with box plots for 20 year time slices. Typical results of downscaled predictand obtained from the predictors are presented in **Figure 3**. In part (i) of **Figure 3**, the precipitation downscaled using NCEP and GCM datasets are compared with the observed precipitation for the study region using box plots. The projected precipitation for 2001–2020, 2021–2040, 2041–2060, 2061–2080 and 2081–2100, for the four scenarios A1B, A2, B1 and COMMIT are shown in (ii), (iii), (iv) and (v) respectively.

From the box plots of downscaled predictand (Figure 3), it can be observed that precipitation are projected to increase in future for A1B, A2 and B1 scenarios. The projected increase of precipitation is high for A1B and A2 scenarios whereas it is least for B1 scenario. This is because among the scenarios considered, the scenario A1B and A2 have the highest concentration of atmospheric carbon dioxide (CO2) equal to 720 ppm and 850 ppm, while the same for B1 and COMMIT scenarios are 550 ppm and  $\approx$  370 ppm respectively. Rise in concentration of CO2 in the atmosphere causes the earth's average temperature to increase, which in turn causes increase in evaporation especially at lower latitudes. The evaporated water would eventually precipitate [10,25]. In the COMMIT scenario, where the emissions are held the same as in the year 2000, no significant trend in the pattern of projected future precipitation could be discerned. The overall results show that the projections obtained for precipitation are indeed robust.

### 8. Conclusions

This paper investigates the applicability of the various linear regression approaches such as direct, forward, backward and stepwise to downscale precipitation from



Figure 2. Typical results for comparison of the monthly observed Precipitation with Precipitation simulated using direct regression downscaling model *M*4 for NCEP data. In the Figure calibration period is from 1990 to 1995, and the rest is validation period.



Figure 3. Box plots results from the direct regression-based downscaling model M4 for the predictand Precipitation.

GCM output to local scale. The effectiveness of this model is demonstrated through the application of lake catchment in arid region in India. The predictand is downscaled from simulations of CGCM3 for four IPCC scenarios namely SRES A1B, A2, B1 and COMMIT. Four regression models are developed and the performance of the models is evaluated using the statistical measures CC, SSE, MSE, RMSE, NMSE,  $\eta$  and MAE. The overall conclusions of this evaluation study are as follows:

1) Overall direct regression performed best followed by backward regression method. Backward regression was followed by forward regression and stepwise regression which yielded the similar results.

2) Direct regression yielded better results for training data set while forward regression performed better for validation data set.

3) The results of downscaling models show that precipitation is projected to increase in future for A2 and A1B scenarios, whereas it is least for B1 and COMMIT scenarios using predictors.

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# **Modeling of Asphaltene Grading in Oil Reservoirs**

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### ABSTRACT

Reservoir fluids frequently reveal complex phase behaviors in hydrocarbon columns owing to the effects of gravity, thermal diffusion, biodegradation, active charging, water washing, seals leaking, and so on. In addition, the formation compartmentalization often causing discontinuous distributions of fluid compositions and properties makes the proper fluid characterization and reservoir architecture even more challenging yet compelled. The recognition of compositional grading and flow barriers becomes a key to accurate formation evaluation in a cost effective manner. Downhole fluid analysis (DFA) of asphaltene gradients provides an excellent method to delineate the complexity of black oil columns. In this paper, a methodology was developed to estimate downhole asphaltene variations with depths using an equation-of-state (EOS) approach coupled with DFA measurements. DFA tools were used to determine fluid compositions of  $CO_2$ ,  $C_1$ ,  $C_2$ ,  $C_3$ - $C_5$ ,  $C_{6+}$ , gas-oil ratio (GOR), density and the coloration (optical density) associated with asphaltene contents at downhole conditions. The delumping and characterization procedures proposed by Zuo et al. (2008) were employed to obtain the detailed compositions excluding asphaltenes. In addition, a molar mass distribution of asphaltenes was described by a three-parameter Gamma probability function. The Gaussian quadrature method was used to generate asphaltene pseudocomponents. Five pseudocomponents were employed to represent the normal asphaltene nanoaggregates. Asphaltene distributions in oil columns were computed by tuning the molar mass of asphaltene nanoaggregates against the DFA coloration logs at a reference depth. The methodology was successfully applied to investigate black oil reservoir connectivity (or flow barriers) for offshore field cases. The analysis results were consistent with the subsequent production data and analytical chemistry. Furthermore, for simplicity, it is reasonable to assume that asphaltenes have average properties such as molar mass in entire oil columns. The results obtained in this work demonstrate that the proposed method provides a useful tool to reduce the uncertainties related to reservoir compartmentalization and to optimize the DFA logging during acquisition.

Keywords: Reservoir Connectivity, Asphaltene Gradients, Equations of State, Downhole Fluid Analysis

### 1. Introduction

In the past few decades, fluid homogeneity has often been assumed in a reservoir. Reservoir fluids frequently reveal complex phase behaviors in single oil columns owing to gravity, thermal gradients, biodegradation, active charging, water washing, seals leaking, and so on. In addition, reservoir compartmentalization often leads to discontinuous compositional distributions at least of one fluid analyte, which is the biggest risk factor in deepwater oil production. A density inversion (higher density fluids are in the shallower oil column) usually implies a likely sealing barrier. Knowing actual fluid profiles in the reservoir enables identification of corresponding compartments. Consequently, the family of DFA measurements is expanding in part to enable greater efficacy in reservoir characterization. Consequently, identifying continuous fluid gradients in the reservoir provides a method to suggest connectivity of the reservoir. In particular, since continuous gradients are generally produced by time dependent mechanisms, the existence of fluid gradients implies connectivity albeit with an unknown time scale. Nevertheless, if considerable fluid flow is required to yield such a gradient, this suggestion of connectivity is much more powerful than that of pressure communication where little fluid flow is required. In particular, if the asphaltenes are observed to have been equilibrated across a reservoir, laterally and vertically, this is a strong connectivity because 1) asphaltenes necessarily charge into the reservoir in a much nonequilibrated state and 2) to equilibrate the component of crude oil with by far the least mobility necessitates substantial permeability. We note that measurements of fluid gradients are a far better way to detect connectivity than measurement of homogeneous properties of a fluid. One could easily imagine a single reservoir charged with a homogeneous fluid, where the reservoir subsequently develops a sealing barrier either from compaction or faulting. Maintaining continuous gradients in evolving separate compartments is much harder to justify. DFA has been used to measure continuous fluid profiles and stair-step discontinuous fluid properties addressing reservoir connectivity and compartmentalization. Fluid compositional variations are very useful to identify sealing barriers or compartments in hydrocarbon columns [1,2].

Downhole fluid analysis (DFA) measurements provide a useful tool to determine the insitu compositional gradients in real time. Recently, Zuo et al. [3] integrated the equation of state (EOS)-based DFA log predictions with DFA measurements to delineate the complexity of reservoir fluids and reservoir architecture. This methodology is the most suitable for the reservoirs that exhibit significant compositional grading of at least one chemical analyte. As mentioned by Hoier and Whitson [4] and Mullins [5], for equilibrium fluid distributions, the variations of fluid compositions and properties are usually small with depth if the reservoir conditions are far away from the critical point and the saturation point (e.g. highly undersaturated black oil). This especially applies to the alkane distributions [5]. For example, a case study showed that in an undersaturated black oil reservoir, the gas-oil ratio (GOR) and compositional gradients were small for large sand bodies in Gulf of Mexico (GoM) [1,2]. Nevertheless, the asphaltene gradient was rather substantial considering the 1000 meters vertical offset of the tilted sheet reservoir. The flow connectivity in the reservoir might not be identified according to the information of bulk fluids such as compositions, GOR and density. Fortunately, the DFA tools not only measure bulk fluid properties like compositions of C<sub>1</sub>, C<sub>2</sub>, C<sub>3</sub>-C<sub>5</sub>, C<sub>6+</sub> and CO<sub>2</sub>, GOR and density but also coloration which is associated with asphaltene contents.

Asphaltenes are defined by a solubility classification, for example, soluble in toluene, insoluble in n-heptane. The asphaltenes are the heaviest components of crude oils with the least diffusivity and have the greatest grading with depth due to a gravitational force. In the cases shown by Mullins *et al.* [1], Betancourt *et al.* [2] and Indo *et al.* [6], the detailed DFA and laboratory analyses of asphaltene contents indicated the evident asphaltene gradient with depth while the resin gradients are much smaller than asphaltenes. The asphaltenes are dispersed in crude oils as nanoaggregates. This information pro-

vides us a new powerful method of determining flow connectivity (barriers) in the reservoir by measuring asphaltene (coloration) contents with depth at downhole conditions, especially when bulk fluid property and compositional gradients are not observable.

Continuous and equilibrium asphaltene gradients have been observed in deepwater oil fields [1,2,7]. In order to establish the asphaltene gradient that is in equilibrium, it is required to establish the colloidal nature of asphaltenes in crude oil [1]. It has been established that asphaltenes are nanocolloidally dispersed in a laboratory setting as well as a field setting. We note that higher aggregation (a cluster of nanoaggregates) exists in the reservoir for either large asphaltene mass fractions such as heavy oils and/or unstable crude oils, but there is a class of black oils with asphaltenes dispersed as ~2nm nanoaggregates. With this knowledge equilibrium distributions of asphaltenes across a field can be established. Asphaltenes in reservoir crude oils, dispersed as asphaltene nanoaggregates, have by far the lowest rate of diffusion compared to any crude oil components. Consequently, when they are in equilibrium throughout a column, then massive fluid flow is indicated thereby positively constraining connectivity. Nevertheless, the time frame is still unknown in these novel analyses. Still the constraint indicates greater connectivity than simply pressure communication which requires almost no fluid flow at geological time scales.

Current DFA tools can measure the coloration of reservoir fluids which is associated with the asphaltene contents. Mullins *et al.* [1] developed a method to calculate asphaltene gradient combining DFA data with the Boltzmann gravitational equation. However, as mentioned by Hirschberg [8], the Boltzmann equation is valid only for ideal solutions. The non-ideality should be taken into account by either the activity coefficient model like a Flory-Huggins type solubility model or the EOS.

Up to now, no one has applied EOS approach to describe an asphaltene gradient in reservoirs although there have been a lot of publications on modeling asphaltene precipitation (onset) using EOS approach in the open literature except for work in the references [9]. Following the traditional EOS approach which has been broadly used for modeling reservoir fluids, Nghiem et al. [10,11] arbitrarily split the heaviest component (C<sub>31+</sub> fraction) in the crude oil into two parts: non-precipitating and precipitating components. The precipitating component was considered to be an asphaltene component. Qin et al. [12] implemented the model of Nghiem in their compositional model. They treated asphaltenes as a pure component with the same critical properties as heavy hydrocarbons, except for the binary interaction parameters. Pedersen and Christensen [13] treated the aromatic fraction of  $C_{50+}$ 

as asphaltenes. The authors mentioned above assumed that asphaltenes are monomers and part of C<sub>n+</sub> fraction (e.g,  $C_{31+}$ ,  $C_{36+}$ ) in crude oils, which is contradicted with the recent observations in advanced asphaltene science that asphaltenes are dispersed as nanoaggregates in crude oils [1,2,6]. Most recently, the EOS approach was employed to account for the nonideality of oils [9] and a methodology for interpreting downhole fluid analysis was developed for estimating downhole asphaltene variations with depth. The methodology can be integrated into the new workflow [3,9,14] as one useful analysis means in analyzing asphaltene coloration gradients. However, the EOS approach developed by Zuo et al. [9] treated asphaltenes to be a single pseudocomponent which is too simple because asphaltenes are defined as the crude oil components soluble in toluene but insoluble in n-alkanes such as n-heptane. The asphaltenes are mixtures which have components in a wide range of molar masses. Therefore, distribution functions and proper characterization of asphaltenes are highly demanding to describe asphaltene components in the EOS approach.

In this work, the EOS approach was employed to account for asphaltene gradients in reservoirs. A three-parameter Gamma distribution function was used to describe asphaltenes. Two field case studies were presented. The results in both case studies were proved by the subsequent production data and analytical chemistry. The results show that the developed methodology can be integrated into the new workflow [14] as one useful means in analyzing asphaltene coloration gradients and in discerning reservoir connectivity.

# 2. Asphaltene Molar Distributions and Asphaltene Characterization

Recently, Pomerantz et al. [15] determined molar mass distributions of asphaltene monomers using two-step laser mass spectrometry. The results show that petroleum asphaltenes without aggregation have a peak at every nominal mass under an envelope beginning at 200 g/mol, peaking at ~600 g/mol and extending to 1000~1500 g/mol. Mullins et al. [16] reviewed the open literature on asphaltene molar mass measured by different methods and concluded that petroleum asphaltenes have a number average molar mass of ~750 g/mol (± 200 g/mol) with a range of 500-1,000 g/mol. As mentioned by Mullins in his new book [17] and the references [1,2], asphaltenes are dispersed in crude oil as nanoaggregates with 4~10 monomers and ~2 nm in diameter. Hence, the molar masses of asphaltenes in black oil are in a range of 500-7,500 g/mol from molecules to nanoaggregates (precluding clusters). On the other hand, asphaltenes may differ at different depths because asphaltenes are defined as a solubility class. Therefore, distribution functions are

required in characterizing asphaltene components in the EOS approach because a single component may not be good enough for asphaltenes.

The three-parameter Gamma function is chosen for describing molar mass distribution of asphaltene nano-aggregates [18-20]. The probability density function, p(x), is given by

$$p(x) = \frac{\left(x - M_{\min}\right)^{\alpha - 1} \exp\left[-\left(x - M_{\min}\right)/\beta\right]}{\beta^{\alpha} \Gamma(\alpha)}$$
(1)

where  $\alpha$ ,  $\beta$  and  $M_{min}$  are the three parameters defining the distribution.  $M_{min}$  can be set to the average molar mass of asphaltene monomers [16] for asphaltene nanoaggregates since it represents the minimum molar mass to be included in asphaltene nanoaggregates (e.g., 500 g/mol). If  $\alpha$  is given,  $\beta$  can be estimated by

$$\beta = \frac{\left(M_{avg} - M_{\min}\right)}{\alpha} \tag{2}$$

The parameter  $\alpha$  can be determined by fitting experimental data of asphaltene distributions. For most asphaltenes and bitumens,  $\alpha = 3.5$  is suitable [21]. Therefore, the average molar mass of asphaltene nanoaggregates is only one adjustable parameter in the distribution function, which can be determined by matching the DFA color gradient data in oil columns. The average molar mass of asphaltene nanoaggregates is adjusted to match DFA color gradient data (typically,  $M_{avg} = \sim 2,000$  g/mol) with  $\sim 2$  nm in an average diameter.

The Gaussian quadrature method is used to discretize the continuous Gamma distribution using N quadrature points [19]. Number of pseudo-components (N) can be from one to 30 for representing asphaltenes (typically 5).

The asphaltene molar mass distribution function can be incorporated into the generalized asphaltene gradient formula described below using the equation of state (EOS).

### 3. Generalized Formula for Compositional and Asphaltene Grading with Depth

Compositional grading in reservoir columns has been studied by many researchers [3,4,22,23] since 1980s. For a mixture of reservoir fluids with *N*-components, a set of mass flux equations for all components are expressed as

$$J_{i} = J_{i}^{Chem} + J_{i}^{Grav} + J_{i}^{Therm} + J_{i}^{Pres} \quad i = 1, 2, ..., N, \quad (3)$$

where  $J_i$  is the mass flux of component *i*. The superscripts *Chem*, *Grav*, *Therm* and *Pres* stand for the fluxes owing to chemical, gravitational, thermal and pressure forces, respectively.

To calculate compositional gradients with depth in a hydrocarbon reservoir, it is usually assumed that all the components of the reservoir fluids have zero mass flux, which is a stationary state in absence of convection [4]. At the stationary state, the fluxes in Equation (3) are equal to the external flux at the boundary of the system. The external flux could be an active charge [22],  $J_i^e$ . It is assumed that the external mass flux is constant over the characteristic time scale of filing mechanisms in the formation.

By taking into account the driving forces due to chemical, gravitational, pressure, thermal impacts and the external flux, the resulting equations are given by

$$\sum_{j=1}^{N} \left( \frac{\partial \mu_{i}}{\partial n_{j}} \right)_{T,P,n_{j\neq i}} \nabla n_{j} - \left( M_{i} - \overline{\nu_{i}}\rho \right) g + \frac{F_{Ti}}{T} \nabla T + \frac{J_{i}^{e} RT}{x_{i}\rho D_{i}} = 0,$$
  
$$i = 1, 2, \dots, N$$
(4)

where  $\mu_i$ ,  $x_i$ ,  $v_i$ ,  $M_i$ ,  $D_i$ , g, R,  $\rho$  and T are the chemical potential, the mole fraction, the partial molar volume, the molar mass and diffusion coefficient of component *i*, the gravitational acceleration, universal gas constant, the density, and the temperature, respectively.  $F_{Ti}$  is the thermal diffusion flux of component *i* and  $n_j$  is the mole number of component *j*.

The thermal diffusion flux of component  $i (F_{Ti})$  can be calculated by the different thermal diffusion models. An example is the Haase expression [23]

$$F_{Ti} = M_i \left( \frac{H_m}{M_m} - \frac{H_i}{M_i} \right)$$
(5)

where subscripts *m* and *i* stand for the property of the mixture and component *i*, respectively. *H* is the molar enthalpy. Pedersen and Lindeloff [23] developed expressions for calculating enthalpy. However, the values of ideal gas enthalpy for  $C_3$  and  $n-C_4$  are determined by optimizing absolute ideal gas enthalpy at 273.15 K and that for  $C_1$  was arbitrarily set to zero. The *H* values can be treated as adjustable parameters for pseudo-components to match DFA data in this work. The chemical potential is calculated through the calculation of fugacity. The resulting equations are given by

$$\Delta \left( \ln f_i \right) - \frac{M_i g \Delta h}{RT} + M_i \left( \frac{H_m}{M_m} - \frac{H_i}{M_i} \right) \frac{\Delta T}{T} + \frac{J_i^e}{x_i \rho D_i} = 0,$$
  
 $i = 1, 2, ..., N$ 
(6)

where  $f_i$  is the fugacity of component *i* and *h* stands for the vertical depth. An EOS can be used to estimate the fugacity of component *i*.

The critical properties, acentric factors of components are required for the EOS to calculate fugacity coefficients. The delumping and characterization procedures of Zuo and Zhang [24] and Zuo *et al.* [25] are applied to characterize single carbon number and plus fractions of reservoir fluids at a reference depth. The asphaltene components are characterized by the method described in the previous section. The EOS is used to estimate fugacity. The DFA and/or PVT data are matched by tuning the EOS parameters to establish a reliable fluid EOS model. The compositions at depth h are obtained by solving Equation (6) numerically based on the data at the reference depth.

In the reference [9], the EOS was used to estimate asphaltene grading (profiling) in oil columns. However, asphaltenes are simply treated to be a single pseudocomponent. It is known that asphaltenes are a mixture whose molar masses vary over a wide range. Therefore, the asphaltene molar mass distribution function mentioned previously is introduced into the EOS approach. By doing this, everything is kept the same as described in the reference [9] but asphaltenes are treated as multiple pseudocomponents using the molar mass distribution function documented in the previous section to obtain mole fractions and molar masses.

The properties of the asphaltene pseudocomponents such as their critical temperatures ( $T_c$ ) in K, critical pressures ( $P_c$ ) in atm and acentric factors ( $\omega$ ) are computed by the correlations in terms of asphaltene molar masses. It is assumed that asphaltene properties follow the same trend as the pseudocomponents. The correlations were then obtained by fitting the pseudocomponent data characterized by the procedures of Zuo and Zhang [24] and Zuo *et al.* [25] for more than 10 different crude oils. The correlation are given by

$$P_{ci} = 53.6746 M_i^{-0.2749} \tag{7}$$

$$T_{ci} = 173.3101 \ln M_i - 439.9450 \tag{8}$$

$$\omega_i = 0.343048 \ln M_i - 1.26763 \tag{9}$$

The density of asphaltene pseudocomponents in  $kg/m^3$  can be calculated by the expression from [26,27]

$$\rho_i = 670 M_i^{0.0639} \tag{10}$$

where  $M_i$  is the molar mass of asphaltene pseudocomponent *i*. We can also set it as a fixed value of 1200 kg/m<sup>3</sup> for all asphaltene pseudocomponents as done by Mullins [1] and Wang and Buckley [28].

The asphaltene properties are dependent on molar mass and density just like typical hydrocarbon pseudocomponents. The volume translation parameter is estimated by matching the specific gravity of asphaltene components at standard conditions.

### 4. Results and Discussions

### Case 1

The Tahiti field was studied by Betancourt et al. [2] and

Mullins *et al.* [1] using the Boltzmann distribution equation. The reservoir has a 1,000-m vertical column of inhighly undersaturated black oil with GOR in a range of f 90 to 116  $m^3/m^3$ , which slightly decreases with depth. in The formation has two main sands: M21A and M21B, but are not in pressure communication, so are not in flow communication. Pressure communication is a necessary to but not sufficient condition to establish flow communication.

odology proposed in this work. The composition (analyzed to  $C_{30+}$ ) as well as saturate, aromatics, resin, and asphaltene (SARA) analysis data were measured at different depths in the laboratory. The laboratory-measured compositions were then lumped into the DFA-like five components/groups (CO<sub>2</sub>,  $C_1$ ,  $C_2$ , C3-C5 and C6+, referred to as pseudo-DFA data). The weight percentages of the five lumped components/ groups were the inputs of the EOS model. The SARA analysis and the DFA coloration (optical density, OD) data were applied to determine the relationship between asphaltene contents in stock-tank oil (STO) and DFA coloration measured at downhole conditions. The linear relation was obtained by Betancourt *et al.* [2]: OD = 0.38 $\times$  wt% + 0.0059, with a small offset at the origin due to some coloration of the resin fraction.

tion. However, pressure is in communication in each primary sand body. The case was used to test the meth-

Based on the compositions of the five lumped components/groups and asphaltene content at a relative depth of 1,555 m in the M21B sand (reference DFA station), as well as the delumping and characterization method of Zuo *et al.* [25], the pseudo-DFA data were delumped and characterized to full  $C_{30+}$  compositions. The delumped composition is compared with the gas chromatography (GC) data as shown in **Figure 1**. The agreement is good between the deplumed and GC data. The physical properties and binary interaction parameters were generated which are required in the EOS calculation.



Figure 1. Comparison of GC and delumped compositions at the reference depth for Case 1. The delumped compositions are in good agreement with the GC data. The delumped compositions are used as inputs to the asphaltene gradient analysis.

The predicted phase envelope of this fluid as depicted in **Figure 2** indicates the formation condition is far away from its critical and bubblepoints (the formation pressure is ~1400 bar). According to the observation of Hoier and Whitson [4], it is expected that the fluids have slight compositional and property grading with depth because the fluids are hardly compressible and highly undersaturated.

It is assumed that the reservoir is isothermal and there is no external flux. Compositional gradients with depth were estimated in terms of the pseudo-DFA data at a relative depth of 1,555 m (reference depth) by solving Equation (6) without external fluxes and temperature gradients. The predicted formation and bubblepoint pressures are compared in **Figure 3** with the pretest and laboratory data. The results show that the predicted formation and bubblepoint pressures agree very well with the measurements.



Figure 2. Phase envelope for fluid in Case 1. The predicted bubble point is close to the experimental data. The formation conditions (P = ~1400 bar) is far away from the critical and bubble points. Slight compositional gradients are expected according to the Hoier and Whitson [4] theory.



Figure 3. Comparison of predicted and measured bubble point and formation pressure for Case 1. The predictions are in accord with the measurements. The formation pressures are much higher than the bubble points. Slight compositional gradients are anticipated according to the Hoier and Whitson [4] theory.

The predicted compositions are compared with the measurements as shown in **Figure 4**. Good agreement is obtained between the measurements and the predictions.

The compositional gradients of the reservoir fluids with depth are small in the Tahiti reservoir. Therefore, it is difficult to determine whether the fluid is in equilibrium or in different compartments using the traditional compositional grading method [3] because the variation of bulk fluid properties (except asphaltenes) is not evident. However, the asphaltene gradient in the column can be used for determining whether the reservoir is in equilibrium or is disconnected because asphaltenes are the heaviest components in crude oil and appear in nanoaggregates (<10 monomers). In the equilibrium model, asphaltenes have the greatest grading in crude oil owing to a gravitational segregation, although other components do not have significant gradient with depth. Furthermore, asphaltene contents are usually low in crude oil and have little impact on the bulk fluid properties such as GOR, light-end composition, and/or density. As viscosity soon joins the pantheon of DFA measurements, asphaltene content can be crosscorrelated to viscosity.

Since the Tahiti fluids are highly undersaturated black oil with very high formation pressure (~1400 bar) which is much greater than asphaltene onset pressure and relative low asphaltene content (<5 wt%), there is no asphaltene precipitation/deposition (*i.e.*, asphaltenes are stabilized) at downhole conditions. Therefore, there exist no clusters of asphaltene nanoaggregates but asphaltene nanoaggregates. The average molar mass of the asphaltene nanoaggregates in the distribution function at the reference depth was adjusted to match the coloration variation data measured by DFA. The adjusted average molar mass of the asphaltene nanoaggregates is 1,602 g/mol corresponding to ~2 nm in diameter.

**Figure 5** shows the predicted optical density (OD) variations and DFA measurements with depth. The results are similar to those obtained by Betancourt *et al.* [2] using the Boltzmann distribution equation. The coloration analyses also indicate that the sands of M21A (center), M21A North, and M21B are in different compartments. In the paper of Betancourt *et al.* [2], detailed discussions were given with regard to reservoir connectivity and coloration log predictions. The ideas are employed in this work as well.

The same fitted molar mass of the asphaltene nanoaggregate component is suitable for the entire reservoir. This means that asphaltenes have the same average size in nanoaggregates in the oil column. Most of the data from the field lies on the theoretical fit curves obtained from the EOS model of asphaltene nanoaggregates. The GOR of the crude oil is low so relatively uniform. Therefore, the entire field has the same asphaltene gradient, but



Figure 4. Compositional variations with depth for Tahiti fluids in Case 1. The predictions are in good agreement with the experimental data. The compositional gradients are small with depth, which has confirmed the Hoier and Whitson [4] theory.



Figure 5. Optical density variations with depth for Case 1. The lines denote the EOS calculations using an average asphaltene molar mass of 1602 g/mol. The symbols stand for the measurements by Live Fluid Analyzer (LFA). Sand M21A is disconnected with Sand M21B. Sand M21A North is not connected with main Sand M21A. The subsequent production data confirmed that the reservoir connectivity is implied when the reservoir asphaltenes are in equilibrium.

the north part of M21A has a much lower asphaltene concentration than the south and centric parts of M21A. As mentioned by Betancourt *et al.* [2], after a careful review of the seismic data, it is plausible that the north part of M21A is disconnected from the M21A sand (center). The M21B sand is in a different compartment than the M21A sands as determined by the formation pressure gradient and geochemistry fingerprinting of the crude oil samples; the coloration analysis is consistent in this assessment, as seen in **Figure 5**. The subsequent production data from this field confirmed that the reservoir connectivity is implied when the reservoir asphaltenes are in equilibrium.

### Case 2

Recently, Betancourt *et al.* [7] reported that black oil in a 200-m vertical column was analyzed by DFA and advanced laboratory analytical chemistry methods. The

oil samples were taken from two wells with low and similar GOR of ~125  $m^3/m^3$ ; the shallower sample PER-1 is from a depth of x674 m, the deeper sample PER-2 is from x874 m. This is also highly undersaturated black oil whose critical point and bubble point is far away from formation conditions. The asphaltene content in stock tank oil (STO) was analyzed by a standard n-heptane precipitation method. This case was also used to test the methodology proposed in this work. Similar to the Tahiti field, the compositional and property gradients are small according to both the laboratory measurements and the EOS model. The fluids are highly undersaturated and rather incompressible; therefore, the hydrostatic head pressure in the reservoir does little to impact a compositional variation. Instead of the absolute pressure, it is the relative pressure difference in the 200-m vertical column of oil that plays an important role in generating gradients. It is impossible to conclude whether or not the oil column is connected in terms of the traditional compositional grading method. Again, coupling the asphaltene gradient analysis with the other advanced chemical analyses could give a conclusion.

If it is assumed that the reservoir is isothermal and there is no external flux, the average asphaltene molar mass is adjusted to the DFA coloration data. The adjusted value is 2070 g/mol. Figure 6 shows coloration variations with depth. The EOS coloration analysis shows the sands in the oil column are connected and the black oils are in equilibrium. The two sands were shown to be in pressure communication, a necessary but insufficient condition to establish flow communication on production time scales. The two black oils have similar low GORs, which is consistent with their being in equilibrium. Furthermore, the reservoir sand properties are consistent with the contained fluids being in equilibrium. The primary reservoir sand has permeability of ~ 1 darcy, which favors convective mixing (much faster than diffusive mixing). These conditions are very similar to those in the Tahiti reservoir, which also appeared to be in equilibrium. The other advanced chemical analyses gave the same conclusion as described by Betancourt et al. [7].

**Figure 7** shows the molar mass distribution of asphaltenes at the top and bottom of sands for both case studies. It can be seen that more heavy asphaltenes distributed at the bottom of sands in both cases. Nevertheless, the distribution changes are relatively slight even in a reservoir with as much as ~1000 m vertical depth. Therefore, for simplicity, it is reasonable to assume that asphaltenes have average properties such as molar mass in entire oil columns.

### 5. Conclusions

This paper presented a methodology to analyze asphaltene



Figure 6. Optical density variations with depth for Case 2. The solid line represents the EOS calculation using an asphaltene average molar mass of 2070 g/mol at the reference depth. The squares are the measurements by Live Fluid Analyzer (LFA). The equilibrium nanoaggregate asphaltene profiling indicates that the reservoir is connected. The results are confirmed by the advanced chemical analysis (2-D GC) as shown in [7].



Figure 7. Molar mass distributions of asphaltenes for both Cases I and II. The bottom of reservoirs consists of more heavy asphaltenes than the top. The reservoir vertical thickness is ~1000 m in Case I and ~200 m in Case II. Both cases show variations of average asphaltene molar masses from top to bottom are small. For simplicity, it is reasonable to assume that asphaltenes have average properties such as molar mass in entire oil columns.

grading with depth using the EOS approach and the DFA tools. The inputs are the DFA measurements such as  $CO_2$ ,  $C_1$ ,  $C_2$ ,  $C_3$ – $C_5$ ,  $C_{6+}$ , and the coloration associated with asphaltene contents. The delumping and characterization procedures proposed by Zuo *et al.* (2008) were applied to obtain the detailed compositions including asphaltenes and the parameters of the EOS model. Fluid-profile and coloration logs were computed by tuning the molar mass of asphaltenes against the DFA coloration logs. The methodology has been successfully applied to two cases. The results obtained in this work demonstrate that the proposed method provides a useful tool to reduce the uncertainties related to reservoir compartmentalization and to optimize the DFA logging during acquisition.

In addition, the results show that the treatment of part

of the  $C_{n+}$  fraction as an asphaltene component (monomer) in the traditional cubic EOS approach is contradicted by the recent observations that asphaltenes are dispersed as nanoaggregates in crude oils. For simplicity, it is reasonable to assume that asphaltenes have average properties such as molar mass in entire oil columns.

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# **Combined Generalized Hubbert-Bass Model Approach to Include Disruptions When Predicting Future Oil Production**

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### ABSTRACT

In a previous study [1] the authors had developed a methodology for predicting global oil production. Briefly, the model accounted for disruptions in production by utilising a series of Hubbert curves in combination with a polynomial smoothing function. Whilst the model was able to produce predictions for future oil production, the methodology was complex in its implementation and not easily applied to future disruptions. In this study a Generalized Bass model approach is incorporated with the Hubbert linearization technique that overcomes these limitations and is consistent with our previous predictions.

Keywords: Generalized Bass Model, Hubbert Curve, Oil Production

### **1. Introduction**

It has been reported that world oil production will peak between 1996 and 2048 [2-16]. Typically, the modelling analysis is based on the Hubbert curve, which is defined as:

$$\frac{dQ(t)}{dt} = rQ(t) \left( 1 - \frac{Q(t)}{Q_T} \right), \tag{1}$$

where Q(t) is cumulative production,  $Q_T$  is the ultimately recoverable resource (URR), defined as the sum of all historical and future production, r is a rate constant, and tis time. Equation (1) can be integrated to obtain:

$$Q(t) = \frac{Q_T}{\exp\left(-r\left(t - t_p\right)\right) + 1},$$
(2)

where  $t_p$  is the year when annual production is expected to peak. Differentiation of Equation (2) gives:

$$\frac{dQ(t)}{dt} = rQ_T \left[ \frac{\exp\left(-r\left(t - t_p\right)\right)}{\left[1 + \exp\left(-r\left(t - t_p\right)\right)\right]^2} \right].$$
 (3)

The Hubbert curve, as described by Equation (3), has been widely used for modelling oil production as the constants r,  $Q_T$  and  $t_p$  can be readily quantified by applying Hubbert linearization techniques to historical production data. The disadvantage with the Hubbert approach, however, is that while it is possible to include disruptions the methodology for doing so is very tedious [1].

A recent alternative to the Hubbert curve is the Generalized Bass model, and is defined as [15]:

$$\frac{d\hat{Q}(t)}{dt} = \hat{Q}_T \left( r_1 + r_2 \frac{\hat{Q}(t)}{\hat{Q}_T} \right) \left( 1 - \frac{\hat{Q}(t)}{\hat{Q}_T} \right) x(\tau), \qquad (4)$$

where  $r_1$  and  $r_2$  are rate constants,  $\hat{Q}_T$  is the URR, and x(t) is an intervention function used to insert a disruption. Equation (4) has the general solution:

$$\hat{Q}(t) = r_1 \hat{Q}_T \left[ \frac{1 - \exp\left(-(r_1 + r_2) \int_0^t x(\tau) d\tau\right)}{r_1 + r_2 \exp\left(-(r_1 + r_2) \int_0^t x(\tau) d\tau\right)} \right], \quad (5)$$

which can be differentiated to obtain:

$$\frac{d\hat{Q}(t)}{dt} = r_1 \hat{Q}_T x(\tau) \left[ \frac{(r_1 + r_2)^2 \exp\left(-(r_1 + r_2) \int_0^t x(\tau) d\tau\right)}{\left[r_1 + r_2 \exp\left(-(r_1 + r_2) \int_0^t x(\tau) d\tau\right)\right]^2} \right].$$
(6)

Guseo *et al.* [15] modelled the intervention function as a summation of disruptions,  $i \in \{1,...,n\}$ :

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$$x(\tau) = 1 + f_1(\tau) + f_2(\tau) + \dots + f_n(\tau), \qquad (7)$$

with each disruption having an exponential form, *i.e.*:

$$f_i(t) = c_i \exp(b_i(t - t_{di})) H(t - t_{di}), \qquad (8)$$

where  $t_{di}$ ,  $b_i$  and  $c_i$  are the commencing year, rate constant and constant of the *i*-th disruption, respectively.  $H(t-t_{di})$  is the unit step function, commencing in year  $t_{di}$ , and is defined as:

$$H(t - t_{di}) = \begin{cases} 0 & , t - t_{di} < 0 \\ 0.5 & , t - t_{di} = 0 \\ 1 & , t - t_{di} > 0 \end{cases}$$
(9)

The advantage of the Generalized Bass model approach is that disruptions can be readily accommodated by the intervention function x(t). However, unlike the Hubbert approach, the generalized Bass model constants  $r_1$  and  $r_2$  are not readily quantified from existing production statistics.

### 2. Results and Discussion

World oil production has been modelled using the Generalized Bass model (GBM), given by Equation (6), with the inclusion of the following three disruptions:

1) 1973, OPEC crisis,

- 2) 1979, OPEC crisis, and
- 3) 1990, collapse of the former Soviet Union (FSU).

In applying the GBM, the functions  $f_i(t)$  have been modified<sup>1</sup> so that they linearly decrease for  $t_r$  years before exponentially decaying back to zero. Mathematically, this is given by:

$$f_{i}(t) = \begin{cases} 0, & t < t_{di} \\ c_{i}(t - t_{di})/t_{ri}, & t_{di} \le t < t_{di} + t_{ri} \\ c_{i} \exp(b_{i}(t - t_{di} - t_{ri})), t_{di} + t_{ri} \le t \end{cases}$$
(10)

Numerical values for the constants, c, b,  $t_d$ , and  $t_r$  were obtained by fitting Equation (10) to the historical data. The actual value of these constants depends on the chosen URR value, as indicated in **Table 1**.

The comparison between the GBM (this study) and the corresponding Hubbert-based model (MHM) by Mohr and Evans [1] for the two URR scenarios is given in **Figure 1**. It can be seen that in both cases the GBM and MHM curves are similar, Quantitatively, for a URR of 2234 Gb (**Figure 1(a**)), the GBM projects a peak in global oil production of 29 Gb/y to occur in 2009; with 90 percent depletion by 2047. The corresponding peak in

Table 1. Fitted values for constants used in Equation (10).

Constant	1973 OPEC crisis		1979 ( cri	OPEC sis	1990 collapse FSU		
$\hat{Q}_{T}$ (Gb)	2234	2734	2234	2734	2234	2734	
<i>c</i> <sub>1</sub> (-)	-0.100	-0.130	-0.240	-0.270	-0.040	-0.065	
$b_{1}(y^{-1})$	-0.015	-0.020	-0.001	-0.001	-0.060	-0.001	
$t_{d1}(\mathbf{y})$	1974	1974	1979	1979	1990	1990	
$t_{r1}(y)$	1	1	4	4	1	1	



Figure 1. GBM and MHM [1] Comparison. (a) URR = 2234 Gb; (b) URR = 2734 Gb.

production for the MHM is 30 Gb/y at 2012; with 90% depletion by 2045. Similarly, for a URR of 2734 Gb (**Figure 1(b**)), the GBM shifted the oil production peak to 2017 at 32 Gb/y, with 90 percent depletion taking place by 2060. By comparison, for the MHM the predicted peak year was 2024 at 34 Gb/y, with 90 percent depletion occurring in 2053.

In producing the Generalized Bass Model predictions, values for the rate constants  $r_1$  and  $r_2$  needed to be determined. Usually, these two terms are varied arbitrarily

<sup>&</sup>lt;sup>1</sup>The original exponential function, Equation (8,9) assumed by Guseo *et al.* [15] had a positive rate constant, *b*, which meant that the disruption, *f*, increased with time. In reality, any disruption must eventually dissipate over time.

until the curve matches the historical data, or fitted using least squares or similar techniques. An alternative approach was applied. Firstly, the following expressions were developed:

$$r_{1} = r \frac{\exp\left(-rt_{p}\right)}{\exp\left(-rt_{p}\right)+1}$$
(11)

$$r_2 = r \frac{1}{\exp\left(-rt_p\right) + 1} \tag{12}$$

which relates  $r_1$  and  $r_2$  to the constants r and  $t_p$ , used in the Hubbert analysis. By doing this, the Hubbert Linearization technique can then be applied to the production data, from 1857 up to the year of the first disruption in 1973, to obtain r and  $t_p$ , and ultimately  $r_1$  and  $r_2$ . From the historical data, r was determined to be 0.075 y<sup>-1</sup>, with  $t_p$  values of 141 and 144 years, for URRs of 2234 and 2274 Gb, respectively. Substitution of these values into Equations (11) and (12) resulted in an  $r_2$  value<sup>2</sup> of 0.075 y<sup>-1</sup>, and corresponding  $r_1$  values of 1.916 and 1.530 x10<sup>-6</sup> y<sup>-1</sup>, URRs of 2234 and 2274 Gb, respectively.

The approach described above has two advantages. Firstly, the use of Hubbert analysis, and in particular the linearization methodology, is adopted to obtain constants  $r_1$  and  $r_2$  for the Generalised Bass model. Secondly, the Generalized Bass Model approach is applied, which is readily able to include disruptions. The use of Hubbert analysis, however, does rely on the validity of Equations (11) and (12) and the justification for the use of these equations is given in appendix 1.

### **3.** Conclusions

The study has demonstrated that a Generalized Bass Model with Hubbert analysis can be used to include disruptions in oil production. The predictions are consistent with previous work based on a more tedious approach of using a combination of Hubbert curves and smoothing functions. The advantage of the new approach is that Hubbert Linearization can be readily applied to obtain values for Generalised Bass model constants based on historical data.

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 $<sup>^{2}</sup>r_{2}$  was only approximately 0.075, in reality it was found to be 0.075- $r_{1}$ , however  $r_{1}$  is very small.

Combined Generalized Hubbert-Bass Model Approach to Include Disruptions when Predicting Future Oil Production 31

### **Appendix 1**

Proof that the derivatives, corresponding to annual production, of the Generalized Hubbert and Bass Models are equal.

The Generalized Bass model is able to account for disruptions by introducing an intervention function, x(t), into the Bass model. Following the same analogy, the Generalized Hubbert Model is defined by introducing an intervention function, x(t), into the Hubbert model, given by Equation (1), in the same way, *i.e.*:

$$\frac{dQ(t)}{dt} = rQ(t) \left(1 - \frac{Q(t)}{Q_T}\right) x(\tau)$$
(A1)

Upon integration it can be shown that:

$$Q(t) = \frac{Q_T}{1 + \exp\left(-r\left(\int_0^t x(\tau) d\tau - t_p\right)\right)}$$
(A2)

and by differentiating, leads to:

$$\frac{dQ(t)}{dt} = rQ_T x(\tau) \left[ \frac{\exp\left(-r\left(\int_0^t x(\tau) d\tau - t_p\right)\right)}{\left[1 + \exp\left(-r\left(\int_0^t x(\tau) d\tau - t_p\right)\right)\right]^2}\right]$$
(A3)

The Generalized Hubbert Model (GHM), can be compared with Equation (5), the Generalized Bass Model (GBM). To do this, Equation (A2) can be multiplied<sup>3</sup> by 1 as:

$$Q(t) = Q_T \left[ \frac{1}{1 + \exp\left(-r\left(\int_0^t x(\tau)d\tau - t_p\right)\right)} \right] \times \left[ \frac{\left[\left(1 + \exp\left(rt_p\right)\right) + \exp\left(-r\left(\int_0^t x(\tau)d\tau - t_p\right)\right) - \exp\left(-r\left(\int_0^t x(\tau)d\tau - t_p\right)\right)\right]}{\left(1 + \exp\left(rt_p\right)\right)} \right]$$
(A4)

Equation (A4) can be rearranged to obtain:

$$Q(t) = Q_T \left[ \frac{1}{1 + \exp\left(-r\left(\int_0^t x(\tau)d\tau - t_p\right)\right)} \right] \times \left[ \frac{\left(\exp(rt_p) - \exp\left(-r\left(\int_0^t x(\tau)d\tau - t_p\right)\right)\right) + \left(1 + \exp\left(-r\left(\int_0^t x(\tau)d\tau - t_p\right)\right)\right)}{1 + \exp\left(rt_p\right)} \right]$$
(A5)

which in turn, can be simplified to become:

$$Q(t) = Q_T \left[ \frac{\exp(rt_p) - \exp\left(-r\left(\int_0^t x(\tau) d\tau - t_p\right)\right)}{\left(1 + \exp\left(-r\left(\int_0^t x(\tau) d\tau - t_p\right)\right)\right)} \right] + Q_T \left[\frac{1}{1 + \exp\left(rt_p\right)}\right]$$
(A6)

To the first term on the rhs of Equation (A6), multiply top and bottom by  $exp(-rt_p)$ , then Equation (A6) becomes:

$$Q(t) = Q_T \left[ \frac{1}{1 + \exp(rt_p)} \right] \left[ \frac{1 - \exp(-r\int_0^t x(\tau) d\tau)}{\exp(-rt_p) + \exp(-r\int_0^t x(\tau) d\tau)} \right] + Q_T \left[ \frac{1}{1 + \exp(rt_p)} \right]$$
(A7)

To the first term on the rhs of Equation (A7), multiply top and bottom by  $r (1 + \exp(-rt_p))$ , then Equation (A7) becomes:

$$Q(t) = Q_T \left[ \frac{r}{\left(1 + \exp\left(rt_p\right)\right) \left(1 + \exp\left(-rt_p\right)\right)} \right] \times \left[ \frac{1 - \exp\left(-r\int_0^t x(\tau) d\tau\right)}{\frac{r \exp\left(-rt_p\right)}{1 + \exp\left(-rt_p\right)} + \frac{r \exp\left(-r\int_0^t x(\tau) d\tau\right)}{1 + \exp\left(-rt_p\right)}} \right] + Q_T \left[ \frac{1}{1 + \exp\left(rt_p\right)} \right]$$
(A8)

To the first term on the rhs of Equation (A8), multiply by 1 expressed in the form  $\exp(rt_p)\exp(-rt_p)$ , then Equation (A8) becomes:

<sup>3</sup>Albeit a rather complicated expression for 1.

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$$Q(t) = Q_{T} \left[ \frac{\exp(rt_{p})}{1 + \exp(rt_{p})} \right] \left[ \frac{r \exp(-rt_{p})}{1 + \exp(-rt_{p})} \right] \times \left[ \frac{1 - \exp\left(-r\left[\frac{r \exp(-rt_{p})}{\exp(-rt_{p}) + 1}\right] + \left[\frac{r}{\exp(-rt_{p}) + 1}\right]\right] \int_{0}^{t} x(\tau) d\tau}{\frac{r \exp(-rt_{p})}{1 + \exp(-rt_{p})} + \frac{r}{1 + \exp(-rt_{p})} \exp\left(-\left[\left[\frac{r \exp(-rt_{p})}{\exp(-rt_{p}) + 1}\right] + \left[\frac{r}{\exp(-rt_{p}) + 1}\right]\right] \int_{0}^{t} x(\tau) d\tau} \right] + Q_{T} \left[\frac{1}{1 + \exp(rt_{p})}\right]$$
(A9)

The first term on the rhs of Equation (A9) is the Generalised Bass model as expressed in Equation (5). This can be demonstrated explicitly, by allowing:

$$\hat{Q}_T = \frac{Q_T \exp\left(rt_p\right)}{1 + \exp\left(rt_p\right)},\tag{A10}$$

$$r_1 = r \frac{\exp(-rt_p)}{\exp(-rt_p) + 1}, \qquad (A11)$$

$$r_2 = r \frac{1}{\exp\left(-rt_p\right) + 1}.$$
 (A12)

Substituing Equation (A10-12) into Equation (A9), produces:

$$Q(t) = \hat{Q}_{T} r_{1} \left[ \frac{1 - \exp\left(-[r_{1} + r_{2}]\int_{0}^{t} x(\tau) d\tau\right)}{r_{1} + r_{2} \exp\left(-[r_{1} + r_{2}]\int_{0}^{t} x(\tau) d\tau\right)} \right] + Q_{T} \left[ \frac{1}{1 + \exp\left(rt_{p}\right)} \right]$$
(A13)

Now, the second term on the rhs of Equation (A13) is the constant<sup>4</sup> Q(0), hence Equation (A13) can be rewritten as:

$$Q(t) = \hat{Q}_{T} \left[ \frac{1 - \exp\left(-[r_{1} + r_{2}]\int_{0}^{t} x(\tau) d\tau\right)}{r_{1} + r_{2} \exp\left(-[r_{1} + r_{2}]\int_{0}^{t} x(\tau) d\tau\right)} \right] + Q(0).$$
(A14)

Finally, substitute Equation (5) into Equation (A14) to obtain:

$$Q(t) = \hat{Q}(t) + Q(0)$$
. (A15)

Since Q(0) is a constant, differentiating Equation (A15), leads to:

$$\frac{dQ(t)}{dt} = \frac{dQ(t)}{dt}.$$
 (A16)

which shows that the annual production for the General-

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ized Hubbert and Bass Models are equal, when the relationships, given by Equations (A10-12), are applied and that the cumulative production curves of the Generalized Hubbert and Bass Models, differ by the constant Q(0).

Note: The Equations (A10-12) can be rearranged to obtain:

$$r = r_1 + r_2 \tag{A17}$$

$$t_{p} = \frac{\ln(r_{2}/r_{1})}{r_{1} + r_{2}}$$
(A18)



Figure A1. Comparison between Generalized Bass and Hubbert models. (a) Annual production; (b) Cumulative production.

<sup>&</sup>lt;sup>4</sup>To see this substitute t = 0 into Equation (A2).

$$Q_T = \hat{Q}_T \frac{r_1 + r_2}{r_2}$$
(A19)

The following example is given to demonstrate that the Generalized Hubbert and Bass models provide equivalent predictions. Arbitrarily let  $r = 0.05 \text{ y}^{-1}$ ,  $t_P =$ 200 y and  $Q_T = 1000 \text{ Gb}$ , then from Equations (A10-12),  $r_1 = 2.27 \times 10^{-6} \text{ y}^{-1}$ ,  $r_2 = 0.05 \text{ y}^{-1}$  and  $\hat{Q}_T = 999.95 \text{ Gb}$ . Suppose there is one disruption in year 150, and that  $t_r = 10$  y, c = -0.5 and b = -0.01 y<sup>-1</sup>. The plots of annual and cumulative production for both the Generalized Hubbert and Bass models are shown in **Figure A1**. It can be seen that annual production is identical, while the cumulative production is different only by a constant value of Q(0) = 0.05 Gb.



# **Modelling Irrigation and Salinity Management Strategies in the Ord Irrigation Area**

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### ABSTRACT

The Ord River Irrigation Area (ORIA) is located within northern Western Australia near the Northern Territory border. Since the beginning of irrigated agriculture in the ORIA the groundwater levels have been continuously rising and are now close to the soil surface in some parts of ORIA in northern Western Australia. The groundwater is now saline throughout most of the ORIA and soil salinity risks are high where the watertables are shallow. This research evaluated irrigation and salinity management strategies for sugarcane and maize crops grown over deep and shallow, non-saline and saline watertables in the ORIA. The LEACHC model, calibrated using field data, was used to predict the impacts of various irrigation management strategies on water use and salt accumulation in the root zone. This study concluded that irrigation application equal to 100% of total fortnightly pan evaporation applied at 14 day intervals was a good irrigation strategy for the maize grown over a deep watertable area. This strategy would require around 11 ML/ha of irrigation water per growing season. Irrigation application equal to 75% of total fortnightly pan evaporation, applied every fortnight during first half of the growing season, and 75% of total weekly pan evaporation, applied on a weekly basis during second half of the growing season, would be the best irrigation strategy if it is feasible to change the irrigation interval from 14 to seven days. This irrigation strategy is predicted to have minimal salinity risks and save around 40% irrigation water. The best irrigation strategy for sugarcane grown on Cununurra clay over a deep watertable area would be irrigation application equal to 50% of the total fortnightly pan evaporation, applied every fortnight during first quarter of the growing season, and irrigation application amounts equal to 100% of total weekly pan evaporation, applied every week during rest of the season. The model predicted no soil salinity risks from this irrigation strategy. The best irrigation strategy for sugarcane over a non-saline, shallow watertable of one or two m depth would be irrigation application amounts equal to 50% of total fortnightly pan evaporation applied every fortnight. In the case of a saline watertable the same irrigation strategy was predicted to the best with respect to water use efficiency but will have high salinity risks without any drainage management.

Keywords: Irrigation Modelling, Salinity Modelling, Saline Shallow Watertable, Irrigation Management, Ord River Irrigation Area

### **1. Introduction**

Hydrological conditions change with the introduction of irrigated agriculture in almost any landscape. Increased accession to groundwater starts at the commencement of irrigated agriculture and over time it brings groundwater levels closer to the soil surface and leads to the development of shallow watertables. Evapotranspiration from increased availability of water from shallow watertables is the main cause of soil salinisation in irrigated areas throughout the world [1] and Australia [2]. Availability of abundant water, low population pressures and lack of awareness of the long term implications of excessive use of water has led to the problems of waterlogging and irrigated salinity in a vast majority of the old irrigation systems of the world. Today because of changing climate, high population pressures, water scarcity and increased awareness of the long term implications of excessive use of water every effort should be made to use this resource optimally to enable more production from less water thus reducing wastage via groundwater accession and runoff.

In the Ord River Irrigation Area (ORIA) in northern Australia (**Figure 1**) the groundwater levels were deeper



Figure 1. Map showing the location of the study area in northern Western Australia.

before clearing the native vegetation for irrigated agriculture. With the introduction of irrigated agriculture, the groundwater levels started rising with increased deep drainage below irrigated fields due to excessive use of irrigation water, and leakage from unlined supply channels and drains servicing the area. The groundwater levels continued to rise at 0.3 to 0.5 metres per year beneath most of the central and northern parts of Ivanhoe Plain over time [4]. Until 1990s the groundwater levels were sufficiently deep to prevent any significant capillary aided evapotranspiration and soil salinsation risks [3]. They are now relatively close to the soil surface in some parts of the Ivanhoe and packsaddle plains (Figure 2). Due to the changed hydrological conditions, the chemistry of groundwater probably changed over time [5]. The shallow groundwater electrical conductivity (EC) varies throughout most of the ORIA with levels ranging from 50 to 2160 mS/m [6]. In some parts of the Ivanhoe and Packsaddle plains, the shallow groundwater salinity (EC) is at extreme levels. Because the groundwater is shallow and saline in the ORIA, the risk of developing soil root

zone salinity is high. Saline watertables shallower than two metre below ground surface often lead to the development of soil root zone salinity [7] and [8].

This study was aimed at evaluating water and salinity management strategies for maize and sugarcane crops grown on Cununurra clay in the ORIA. The impacts of both fresh and saline shallow watertables on the water demands and soil root zone salinity were evaluated through modelling. The objectives were to:

### 2. Ord River Irrigation Area

The ORIA is located at Kununurra in the East Kimberley region of Western Australia near the Northern Territory border (**Figure 1**). It occupies around 16,000 ha along the palaeo-alluvial flood plain of the lower Ord River. The land surface in this irrigation area varies by only about 10 m with the surrounding sandstone and basalt ranges outcropping up to around 400 m above the alluvial plain. Presently Stage 1 of the ORIA consists of around 12,000 ha of irrigated agriculture serviced by approximately 135 km of clay-lined supply channels and



Figure 2. Mean observed watertable depth beneath Ivanhoe and Packsaddle plains between July 2003 and June 2004 [4].

155 km of surface drains. The return flow from flood and furrow irrigation systems discharges back into the lower Ord River.

### 2.1. Climate

The climate of this region is semi-arid with summer monsoonal rains. Around 90% of the annual rain is received between November and March. Average wet-season rainfall (July-June) is around 800 mm but is highly variable. Pan evaporation is around 3000 mm per year [9]. Mean monthly pan evaporation exceeds rainfall throughhout the year except February. The mean minimum and maximum temperatures are around 14°C and 30°C in July and 25°C and 39°C in November.

### 2.2. Ord Soils

The dominant soil types include cracking clays from the Cununurra and Aquitaine families. Levee type soil and sands also exist. The Cununurra clays occur in normal, alkaline and leached phases. Detailed information relating to soils in the Ord River area can be found in [10-12]; and [13]. The normal phase of Cununurra Clay occurs in large areas of the Packsaddle Plain and has a dark colour with medium texture and poor drainage. The alkaline phase consists of imperfect to poorly drained brown clays with fine topsoil and exists in a large area south of the Kimberly Research Station on Ivanhoe Plain. The leached phase occurs in the north and east. It generally has a coarser structure and higher clay content and poor to very poor drainage. Aquitaine soils are bluish-grey to yellow cracking clays and exist in areas subjected to prolonged inundation, such as swamps, and have very poor drainage. Smaller areas of the alkaline and acid phases also occur. Packsaddle loamy sands exist adjacent to the Cununurra clays. These are better drained and well suited to intensive horticultural activities. The light textured Ord loamy sands are located near the river. Sand and gravel beds of the old palaeochannel of the Ord River underlie more than 60 percent of the ORIA. These beds form extensive interconnected aquifers under irri-

### gated areas of the Packsaddle and Ivanhoe plains. **2.3. Main Crops and Irrigation Methods**

To identify irrigable areas in the Ivanhoe and Packsaddle plains, a detailed survey of the area was conducted in 1944. The irrigation development project was implemented in stages. Initially, only five farms on Ivanhoe Plain were released for irrigation in 1962. By 1969, a total of 30 farms (5,540 ha) were released. The irrigated area increased by 200% to around 11,000 ha between 1990 and 1999. More than half of over 100 active farms are small and rely on off-farm income. About 40 farms are large-scale where a variety of crops are grown. The main crops include sugarcane, maize, chickpea, sunflower and horticultural including melons, pumpkin, mangoes, bananas citrus and sandlewood. Recently irrigated sandlewood plantations have increased substantially. Sugarcane introduced during 1990s is one of the major crops in the ORIA and has more than double the water requirements of most other crops [14]. Irrigated crops are generally grown during the dry season when growing conditions are best [15]. The irrigated fields are mostly fallow during the wet season except annual crops such as sugarcane.

The value of the main crops ranges between \$60 and \$80 million per annum. The sugarcane, melons and sandlewood produce the highest values. The average output values per hectare of cropped area range from \$2,500 to over \$17,000. Three high value crops include bananas (\$17,200 per ha), melons (\$13,600 per ha) and pumpkin (\$18,800 per ha). The sugarcane has a relatively

low value (\$4,200 per ha). Although bananas produce the highest per hectare values their production has almost ceased recently. The sandlewood values almost three times the value of sugarcane; increasing areas of sandlewood plantations are indicative of their high returns.

Common irrigation methods are furrow, sprinkler and drip. Intensive tree crops and bananas, grown on sandier soils, are irrigated using sprinkler and drip irrigation methods. The clay soils are better suited for broad acre farming. On these clay soils, the furrow irrigation is used for most broad acre crop production including sugarcane and maize. Fields are laser levelled to a gradient ranging between 1:800 and 1:2,000. The furrow lengths are often 200 m long and rarely longer than 500 m. The beds are mostly 1.8 m wide and 0.16 m high above furrow. The height between the surface water in the water course and the tumble area of the furrow is called irrigation head and typically ranges between 100 and 250 mm. The water supply from the water course to the furrow is through siphon whose diameter ranges between 25 mm and 50 mm depending on the furrow length and water supply rate.

Irrigation interval and application amounts vary depending on crop type, growing stage, weather and farmer. They typically range from one week to more than a month and are not optimal. Usually irrigation application amounts are significantly larger than the required amounts determined based on soil moisture deficit. This results in excessive deep drainage and groundwater accessions and runoff from irrigated fields. This also results in application of irrigations when either too much moisture is still available from an earlier irrigation or the crop is under stress due to insufficient soil moisture.

### 2.4. Irrigation Water Availability

The water allocation for Stage 1 (about 11,000 ha irrigated area) is 350 GL per year. An allocation of 400 GL per year is set for irrigation of new area of about 14,000 hectares in Stage 2. The irrigation water is supplied by constructing a Kununurra diversion dam on the Ord River and M1 supply channel network. The Kununurra diversion dam, a 20 m high structure that forms Lake Kununurra of 101 GL storage capacity, holds water in the Ord River water course for approximately 50 km upstream. The Ord River Dam, located approximately 60 km upstream in the Carr Boyd Ranges, was constructed to store water in Lake Argyle to ensure a reliable supply of irrigation water to the ORIA. The water is released from Lake Argyle and stored in Lake Kununurra which provides the head necessary to divert water to irrigation areas in the ORIA. Water levels in Lake Argyle therefore dictate any restriction policies for water demands.

The average annual water availability from Lake Ar-

gyle is 4257 GL. The Lake Argyle water is diverted for irrigation use, hydropower generation and environmental releases. Currently only about 8 percent of the available water is used for irrigation in Stage 1 of the ORIA. With the introduction of Stage 2 irrigation area the level of use for irrigation is projected to increase to about 17 percent. If all controlled releases such as irrigation, environmental and power generation are included the level of use increases to about 57 percent of the available water. Under a wet future climate increased inflows into Lake Argyle are expected and the annual water availability is projected to increase to about 5110 GL and the relative level of use for controlled releases is projected to reduce to about 50 percent. Under a dry future climate, due to decreased inflows into Lake Argyle, the annual water availability is expected to reduce to about 3320 GL and relative level of water use for controlled releases is likely to increase to about 64 percent of the total available water [16].

The water availability for irrigation is not a major issue in the ORIA since relatively secured supplies are likely to be available in the future for existing Stage 1 and future Stage 2 irrigation areas. In the ORIA an efficient on-farm irrigation water management through an optimal irrigation scheduling is mainly required to maximise crop production and minimise excessive deep drainage. Deep drainage fluxes can vary from negative flux [17] to 119 mm per year [18] under irrigated sugarcane. Reduction in deep drainage fluxes through an optimal irrigation scheduling will help control rising watertables and the development of soil salinity in ORIA.

### 3. Model Description

The LEACHC version of LEACHM was selected for irrigation scheduling and assessing the impacts of various fresh and saline shallow watertables on soil salinity built up when the maize and sugarcane are grown on the Cununurra Clay. This model has previously been used for irrigation scheduling under saline shallow watertable conditions [7] and [8]. LEACHM (Leaching Estimation And CHemistry Model) is one of the more complex and comprehensive models for simulating processes in crop root zones [19]. It can also be categorised as a complex model with respect to its approach to soil chemistry because it considers the independent movement of individual ions, including equilibrating the soil solution phase with the solid phase using precipitation-dissolution of lime and gypsum, significant ionic-pairing, and cation exchange. However it tends to under predict reactive ions.

LEACHC uses a finite-difference solution of the one-dimensional Richard's equation for unsaturated flow.

To approximate the hydraulic conductivity, matric potential and moisture content (K-h- $\theta$ ) relationships, the model uses either the expressions developed by [20] or fits the two-part retentivity functions developed by [21]. If this retentivity function is selected, various regression equations are available [19,22,23] and [24]. In this study the equations developed by [20] were used for estimating soil retention relationships based on input of soil textural properties, bulk density, organic carbon and saturated hydraulic conductivity in various layers of the soil profile. To approximate evapotranspiration the model uses the method of [25]. From the input of weekly pan evaporation totals (P), the model calculates daily potential evapotranspiration (ET<sub>d</sub>). To determine daily potential transpiration (T<sub>d</sub>), ET<sub>d</sub> is multiplied by the crop cover fraction ( $C_{cf}$ ). The equation developed by [26] was used to approximate the crop cover during various growing stages of the maize and sugarcane. The daily potential surface evaporation  $(E_d)$  is the difference between  $ET_d$ and T<sub>d</sub>. The equations used for maize and sugarcane root growth and root density distribution as a function of time in this study are based on those given by [27]. The water uptake rate by the maize and sugarcane roots is approximated by using equation developed by [28].

A number of upper and lower boundary conditions are provided in the model. The upper boundary conditions include ponded or non-ponded infiltration and evaporation or zero flux. The five different lower boundary conditions are: a) fixed watertable depth; b) free draining profile; c) zero flux; d) lysimeter tank; and e) fluctuating watertable. A fixed watertable boundary condition was used for this study. Use of Richard's equation for unsaturated flow assumes that the soil is: homogeneous horizontally, rigid and incompressible, non-hysteretic and iso-thermal, and that there is no preferential flow.

After the solution of Richard's equation for unsaturated flow, including sinks, the movement and distribution of solutes are modelled by solving numerically the convection-diffusion equation (CDE). The model can handle the movement and distribution of Ca, Mg, Na, K, Cl, SO<sub>4</sub>,  $CO_3$ , HCO<sub>3</sub>, H, OH and their major ion pairs.

### 4. Material and Methods

Two experimental sites (**Figure 2**) were selected to collect the field data about soil physical properties; irrigation frequency and application amounts; soil moisture, watertable depth, and soil and water chemistry. The purpose was to monitor temporal changes in soil moisture and salinity profiles over the growing period to assess any water or salt stress under current irrigation practice and calibrate LEACHC to enable its use for evaluating various irrigation management strategies.

### 4.1. Kimberly Research Station Site-KRS 7A

This 6.6 ha site was located near the Kimberly Research Station (KRS) in block 7A (Figure 2). The soil in this block belongs to the Cununurra Clay and a maize crop grown during 2004 was selected for the study. To determine the soil physical and textural properties, soil samples were collected from two locations (7A-1 and 7A-2). At each location, the soil samples were collected from various segments up to 2 m depth. Each soil sample was analysed for soil texture, bulk density, organic carbon, and soil moisture. The saturated paste extracts of soil samples were analysed in the laboratory for major ions, EC and pH. Soil textural and chemical data were used as the initial soil moisture and soil chemical compositions during model calibration. Textural properties of the soil at KRS 7A-1 and KRS 7A-2 (Table 1) were averaged and used as input in the LEACHC model for estimating the soil retention properties. A total soil profile depth of 2 m was divided into 10 segments of 200 mm each segment. The soil textural properties varied across its various segments as listed in Table 1 and so were the estimated retention properties. The soil retention properties estimated by the model were similar to those determined through laboratory experiments by [29] for the Cununurra Clay (Table 2). The amount of soil water available for extraction by the maize plant roots from various segments of a 2 m soil profile was averaged around 220 mm.

Additional soil samples, collected on June 11, 2004, July 12, 2004 and October 08, 2004, were analysed for soil moisture and soil chemical properties (EC and pH) and then compared with model predictions during the model calibration. The watertable in the experimental

block, monitored by taking regular water level readings from an existing bore hole at this site, varied around 4 m below ground surface throughout the growing season and accordingly its depth was fixed at 4 m in the model. A groundwater sample, collected from the bore hole and analysed for major ions, EC and pH, indicated that the shallow groundwater was saline; EC around 400 mS/m (**Table 3**); major ions were used as input in the model to represent the initial chemical composition of the watertable.

The maize was sown during the last week of April 2004 which germinated during the first week of May and developed its full canopy during the last week of July 2004. It was harvested during the first week of October 2004. These dates were used for simulating the maize crop growth in the LEACHC. The fertilizer application rates were 250 kg/ha Di-Ammonium Phosphate (DAP), 50 kg/ha Zinc Sulphate Monohydrate, 50 kg/ha Sulphate of Potash and 460 kg/ha Urea. The maize roots can develop up to 2 m below the ground surface [30]. However most of the maize roots are concentrated within the top parts of the soil profile according to many researchers [31,32] and [33]. For this study a 2 m root zone was assumed. The relative fraction of maximum root length density followed that described by [34]. Using this generic distribution the root zone was subdivided into four quarters with 40, 30, 20 and 10 percent of the roots in each quarter starting from top of the soil profile.

Total irrigation and rainfall amounts applied to the crop and used as input into the model were 1300 mm and 15 mm, respectively during the growing season (**Table 4**). The irrigation applications remained uniform throughout the growing period. During each watering, 9.5 ML was applied in 12 hours to irrigate 6.6 ha of the maize. Because

KRS 7A-1 Depth (mm)	Sand %	Silt %	Clay %	<b>OC</b> <sup>*</sup> %	KRS 7A-2 Depth (mm)	Sand %	Silt %	Clay %	OC* %
0-100	39.2	16.0	44.8	1.1	0-100	35.9	9.7	54.4	1.0
100-200	39.8	10.1	50.1	0.8	100-200	39.2	10.7	50.1	0.8
200-400	36.6	14.9	48.5	0.5	200-400	35.2	12.4	52.4	0.7
400-800	32.5	15.1	52.4	0.4	400-800	38.6	13.1	48.3	0.4
800-1100	36.3	14.2	49.5	0.4	800-1100	36.3	14.4	49.3	0.4
1100-1500	29.6	18.7	51.7	0.3	1100-1500	42.1	14.7	43.2	0.2
1500-1700	31.2	16.4	52.4	0.2	1500-1700	36.7	19.8	43.5	0.8
1700-2000	41.1	16.0	42.9	0.1					

 Table 1. Soil textural properties at KRS 7A-1 and KRS 7A-2 near Kimberley Research Station.

\*Organic carbon.

		Pore water pressure (bars)								
Depth (mm)	Bulk density (g/cm3)	0.001	0.1	0.33	0.67	1	3	15		
		Water content (cm3/cm3)								
0-100	1.40	0.42	0.36	0.32	0.31	0.31	0.27	0.17		
100-200	1.42	0.41	0.35	0.32	0.31	0.31	0.27	0.20		
200-300	1.44	0.39	0.35	0.33	0.32	0.32	0.28	0.22		
300-400	1.48	0.41	0.37	0.34	0.33	0.32	0.29	0.23		
400-500	1.52	0.45	0.40	0.37	0.35	0.34	0.30	0.24		
500-600	1.51	0.43	0.39	0.36	0.34	0.34	0.30	0.25		
600-700	1.51	0.43	0.40	0.36	0.35	0.34	0.30	0.26		
700-800	1.52	0.45	0.41	0.38	0.36	0.36	0.31	0.27		
800-900	1.52	0.47	0.42	0.39	0.37	0.36	0.32	0.27		
900-1200	1.52	0.45	0.41	0.38	0.36	0.36	0.31	0.28		
1200-1500	1.52	0.47	0.42	0.39	0.37	0.36	0.32	0.28		
1500-2000	1.52	0.47	0.42	0.39	0.37	0.36	0.32	0.28		

### Table 2. Soil retention properties of cununurra clay.

Table 3. Groundwater and irrigation water quality.

	Ca	Mg	Na	K	Cl	S	HCO <sub>3</sub>	EC	pН	TDS
				mg/L				mS/m		Mg/L
Groundwater quality at KRS-7A	68	104	495	3	960	19	475	400	7.78	-
Groundwater quality at CUM55	13	16	28	3	27	3	123	46	7.89	-
Irrigation water quality (Diversion Dam)	25	12	20	3	14	3	183	30	8.06	178

Table 4. Irrigation and	rainfall amounts for	the Maize crop a	t KRS-7A
Tuble 4. III guildi and	rannan amounts tor	the maile crop a	

Date	02/05/04	13/05/04	26/05/04	03/06/04	12/06
Irrigation/rainfall (mm)	144	144	144	13.5*	144
Date	27/06/04	14/07/04	25/07/04	07/08/04	19/08/04
Irrigation/rainfall (mm)	144	144	144	144	144

\*Denotes rainfall. Only rainfall amounts of 10 mm or more were used in the model

irrigation water quality was not expected to change in the short term, only three irrigation water samples were collected during cropping season and analysed for major ions, EC and pH. These values were used as input to represent the irrigation water quality in the LEACHC model (**Table 3**). The weather data were obtained from KRS weather station. The daily pan evaporation and

temperature data were used to determine the weekly total pan evaporation and mean weekly temperatures and the amplitudes. **Figure 3** shows the weekly total pan evaporation and maximum and minimum temperature data from KRS weather station between April 2004 and July 2005. For the maize crop these data between April and October 2004 were used.



Figure 3. Total weekly pan evaporation and mean weekly minimum and maximum temperatures at KRS during 2004 and 2005.

The saturated past extracts of the soil samples were analysed in the laboratory for the chemical analysis. The major ions obtained from this analysis of the soil samples collected from KRS 7A-1 and KRS 7A-2 were averaged and used as input in the model to represent the initial chemical composition of the soil profile (**Table 5**). Although LEACHC can handle the movement of all major ions but for this study only EC values as representative of overall salinity, obtained from analysis of the soil samples collected during and after the growing period, were used for model calibration.

### 4.2. Cummings Farm Site-CUM 55

The second site was selected at Cummings farm in block 55 (CUM 55), which has soil type belonging to the

Cununurra clays (**Figure 2**). Sugarcane grown on this block during 2004-05 was selected for the study. To determine the soil physical and textural properties, initial soil samples were collected from various segments of the soil profile up to 2 m depth at two locations (CUM 55-1 and CUM 55-2) immediately before the start of the growing season. The samples were analysed for soil texture, bulk density, organic carbon, soil moisture and soil chemistry (**Table 6**). These properties at the two locations (CUM55-1 and CUM55-2) were averaged and used as input to the LEACHC model for estimating the soil retention parameters. The total amount of soil water available for extraction by the sugarcane plant roots from various segments of a 2 m soil profile was averaged around 210 mm.

Table 5. Major ions used as initial chemical composition of the soil profile for KRS site (maize crop).

Major ions (mg/L)										
Depth (mm)	Na	Mg	S	Cl	K	Ca	нсоз	рн		
0-100	2.9	3.9	20.6	44.9	0.2	4.7	70.2	6.8		
100-200	2.4	1.1	12.6	32.3	0.2	1.0	103.2	7.4		
200-400	3.5	0.8	16.9	64.0	0.2	0.7	128.0	7.9		
400-800	9.2	0.7	29.0	230.0	0.2	0.6	160.3	8.2		
800-1100	15.7	0.8	53.8	414.0	0.2	0.6	157.9	8.3		
1100-1400	24.6	1.4	89.9	701.5	0.2	1.0	126.9	7.8		
1400-1700	12.6	0.6	56.0	272.0	0.2	0.2	186.5	8.3		
1700-2000	10.1	0.5	31.1	227.2	0.2	0.1	196.5	8.4		

	(	CUM 55-1			CUM 55-2				
Depth (mm)	Sand %	Silt %	Clay %	OC* %	Depth (mm)	Sand %	Silt %	Clay %	<b>OC</b> <sup>*</sup> %
0-100	26.0	10.6	63.4	1.12	0-100	23.1	19.3	57.6	0.93
100-200	25.3	16.0	58.7	1.04	100-200	27.2	8.1	64.7	1.16
200-400	27.3	11.5	61.2	0.60	200-400	25.0	14.6	60.4	0.42
400-800	23.4	17.7	58.9	0.47	400-800	23.6	13.6	62.8	0.41
800-1100	22.9	18.8	58.3	0.43	800-1100	25.9	12.2	61.9	0.41
1100-1500	22.2	22.0	55.8	0.53	1100-1500	24.0	13.4	62.6	0.32
1500-2000	22.2	34.1	43.7	0.22	1500-1700	54.9	12.3	32.8	0.15

Table 6. Soil textural properties in Block 55 at CUM 55-1 and CUM 55-2 at Cummings farm.

Additional soil samples, collected on June 11, 2004, July 12, 2004, October 08, 2004, March 12, 2005 and July 01, 2005, were analysed for soil moisture and soil chemical properties (EC and pH) and compared with the simulated data during model calibration. The watertable in the experimental block varied between 3.8 and 4.2 m below ground surface during the simulation period. It was assumed at a fixed depth of 4 m in this study. A groundwater sample, collected from the bore hole, and analysed for major ions, EC and pH, indicated that the shallow groundwater quality was relatively fresh with EC 46 mS/m (Table 3); major ions were used as input into LEACHC to represent the initial chemical composition of the watertable. A sugarcane crop was planted during second week of May 2004. It emerged from the ground during the fourth week of May 2004. The crop developed

full canopy by the second week of August 2004 and its harvest started during the last week of June 2005. Fertilizer application rates were 250 kg/ha DAP, 10 kg/ha Zinc, 15 kg/ha Sulphur and 325 kg/ha Urea. These dates were used in the model to simulate the sugarcane crop growth in the model. A rooting depth of 2 m was assumed for the sugarcane crop. The root zone of 2 m was subdivided into four quarters with 40, 30, 20 and 10 percent of the roots in each quarter starting from top of the soil profile. About 1900 mm (946 ML) was applied through 14 irrigations and around 700 mm was received from rainfall during the growing season (Table 7). The irrigation application amounts varied between 106 and 168 mm (53-84 ML applied as one irrigation to the 50 ha crop). These irrigation application and rainfall data were used as input in the model. The chemical composition of the irrigation

Table 7. Irrigation and rainfall amounts for the Sugarcane crop at CUM 55.

Date	08/05/04	03/06/04	20/06/04	22/07/04	17/08/04	24/09/04	28/10/04
Irrigation/rainfall* (mm)	168	10.5*	120	148	120	120	168
Date	06/11/04	08/11/04	13/11/04	15/11/04	22/11/04	09/12/04	09/12/04
Irrigation/rainfall (mm)	12.5*	15*	106	21.5*	106	144	144
Date	22/12/04	26/12/04	27/12/04	01/01/05	02/01/05	03/01/05	06/01/05
Irrigation/rainfall (mm)	16.7*	13.4*	43.1*	17*	130.2*	42.8*	14*
Date	12/01/05	13/01/05	18/01/05	20/01/05	31/01/05	03/02/05	15/02/05
Irrigation/rainfall (mm)	$20^{*}$	13*	168	24.6*	28.8*	34.1*	140
Date	06/03/05	16/03/05	17/03/05	04/04/05	18/04/05	05/05/05	
Irrigation/rainfall (mm)	33*	52.6*	74*	120	144	120	

\*Denotes rainfall. Only rainfall amounts of 10 mm or more were used in the model.

water (**Table 3**) was used to represent irrigation water quality. The weekly pan evaporation and maximum and minimum temperature data from KRS weather station between April 2004 and July 2005 were used as input in the LEAHC model for calibration of the sugarcane crop (**Figure 3**).

The soil samples collected from various depth segments at CUM55-1 and CUM55-2 before the start of growing season of the sugarcane crop were analysed for chemical composition. The chemical composition at each depth segment from two locations was averaged and used as input in the LEACHC to represent the initial chemical composition of the soil profile (**Table 8**). The EC values obtained from analysis of the soil samples collected during and after the growing period were used for model calibration.

### 5. Results and Discussion

### 5.1. Model Calibration

### 5.1.1. Maize Crop at Kimberly Research Station Site—KRS 7A

To calibrate the LEACHC model for the maize crop, field data about soil textural, physical and chemical properties, crop growth, irrigation amounts and quality, watertable depth and quality, total weekly pan evaporation, mean weekly temperatures, and watertable depth and quality were used. The total soil profile depth considered for modelling was 2 m with 20 segments of 100 mm each. The simulation started on 01/04/04, about one month before the crop sowing date, to enable equilibration of soil moisture in the soil profile before the start of the growing season. The simulation end date was on November 30, 2004, approximately 20 days after the crop was harvested on October 07, 2004.

Soil samples, collected during the growing season and

analysed for soil moisture and soil chemistry, were used for comparison with the model results. The two parameters ( $\alpha$  and  $\beta$ ) in Campbell's equation [20] were slightly adjusted to achieve a reasonable agreement between the observed and predicted soil moisture content and salinity profiles. The comparison between the observed and predicted soil moisture content at three dates; April 27, 2004, July 12, 2004 and October 08, 2004 shows that the agreement between observed and predicted soil moisture was reasonable except in the top layers of the soil profile where the model over-predicted the soil moisture content (Figure 4). The Willmott's d-index [35], a measure of the degree of agreement between the observed and predicted values, was above 0.5. Given the inherent difficulty in estimating the soil retention properties in various layers by either using Campbell's equation or various regression equations, this level of agreement between the observed and predicted water content was viewed as sufficiently accurate for simulating the soil moisture in various irrigation management scenarios.

The predicted soil profile electrical conductivity (EC) at the predicted moisture content was converted to ECe (electrical conductivity of the saturated paste extract) based on field and saturated water content [36] for a meaningful comparison with the observed ECe. The ECe will be termed as EC hereafter for simplicity. The LEACHC tends to under predict reactive ions according to [7] and [8]. For this reason the comparison of the observed and modelled reactive ions was not included in the study. Comparison of the observed and predicted soil profile EC at three different dates shows that the agreement between the observed and predicted EC was good except in one layer located just below the middle of the soil profile where it was under-predicted by the model (**Figure 5**). There was an unusual sudden increase

Table 8. Major ions used as initial chemical composition of the soil profile for CUM55 site (Sugarcane crop).

Major ions (mg/L)								
Depth (mm)	Na	Mg	S	Cl	K	Ca	нсоз	рн
0-100	4.9	2.6	18.0	336	0.2	3.1	80.0	7.4
100-200	3.4	3.2	18.0	324	0.1	4.1	27.4	7.0
200-400	5.1	5.1	21.4	558	0.1	7.8	45.8	6.8
400-800	8.8	7.8	37.2	854	0.1	12.1	56.1	7.0
800-1100	14.4	10.2	48.1	1230	0.2	14.3	70.8	7.2
1100-1400	16.3	11.9	54.8	1418	0.2	17.0	95.2	7.7
1400-1700	9.3	4.7	29.5	678	0.2	6.4	80.2	7.5
1700-2000	30.7	13.6	78.1	2037	0.3	20.4	98.7	7.6



Figure 4. Comparison of the observed and predicted soil profile water content at KRS 7A on 27/04/04 (left), 12/07/04 (middle) and 08/10/04 (right).



Figure 5. Comparison of the observed and predicted soil profile EC at KRS 7A on 27/04/04 (left), 12/07/04 (middle) and 08/10/04 (right).

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45

in the observed EC of this layer at two dates that can not be explained. However, in general, the model did a very good job of predicting the soil profile EC. The Willmot's d-index, a measure of the level of agreement between the observed and predicted EC, was averaged around 0.5. The inability of the model to accurately predict EC of the middle soil layers at one occasion (October 2004) resulted in a lower average d-index. A reasonable agreement between the observed and predicted water content and salinity data suggested that this calibrated model can be used to simulate both water content and salinity profiles for the maize crop grown on the Cununurra clay.

### 5.1.2. Sugarcane Crop at Cummings Site—CUM 55

To calibrate the LEACHC model for the sugarcane grown on Cununurra clay required field data collected from CUM 55 and climate data from KRS weather station were used. The simulated depth and depth segments were the same as for the maize. The simulation started on April 01, 2004, about one month before sowing to enable equilibration of soil moisture in the soil profile before the start of the growing season and ended on July 31, 2005, approximately 40 days after the crop was harvested on June 22, 2005. Slight adjustments to the two parameters ( $\alpha$  and  $\beta$ ) of Campbell's equation [20] were made to achieve a reasonable agreement between the observed and predicted soil moisture content and salinity profiles.

Comparisons between the observed and predicted soil moisture contents, depicted in Figure 6 for three dates during 2004 and Figure 7 for two dates during 2005 show that the agreement between the observed and predicted water content was good except on July 08, 2004, when the model under-predicted the soil moisture content in the middle part of the profile which may be due to the use of an incorrect irrigation event in the model. As expected, both the observed and predicted water contents in the surface layers were relatively drier. In the remaining profile the water content was relatively uniform at most dates. The Root Mean Square Error (RMSE) ranged between 0.01 and 0.03 in various segments of the soil profile. The Willmott's d-index, a measure of goodness of fit, ranged between 0.45 and 0.55, which was reasonable considering the variation of soil structure and physical properties expected in the various soil layers.

Comparison between the observed and predicted soil profile ECs on the three dates during 2004 and two dates during 2005 shows that the agreement between the observed and predicted EC was reasonable (**Figure 8** and **Figure 9**). At some dates (July 08, 2004, March 12, 2005 and July 01, 2005) the model slightly over-predicted EC in the middle layers. The prediction was relatively good in the lower layers of the soil profile at most dates. The predicted EC also was close to the observed EC in the top layers of the soil profile except on April 27, 2004,



Figure 6. Comparison of the observed and predicted soil profile soil moisture content during 2004 on 27/04/04 (left), 11/06/04 (middle) and 08/07/04 (right).



Figure 7. Comparison of the observed and predicted soil moisture content of the soil profile at CUM 55 on 12/03/05 (left) and 01/07/05 (right).



Figure 8. Comparison of the observed and predicted soil profile EC at CUM 55 on 27/04/04 (left), 11/06/04 (middle) and 08/07/04 (right).



Figure 9. Comparison of the observed and predicted soil profile EC at CUM 55 on 12/03/05 (left) and 01/07/05 (right).

2000

when it was over-predicted, and July 01, 2005 when it was under-predicted.

2000

A reasonable agreement between the observed and predicted water content and salinity values suggested that the calibrated model is able to simulate soil moisture content and salinity profiles reasonably well if it is used to devise irrigation management strategies for the sugarcane crop grown on the Cununura clay soil for various watertable depths and salinity conditions.

### 5.2. Model Application

Depth (mm)

### 5.2.1. Irrigation Scheduling of Maize Crop—Deep Watertable

To evaluate various irrigation management strategies for the maize crop grown on Cununurra clay all together six simulations, three irrigation application amounts and two irrigation intervals, were considered. In the first three, irrigation application amounts equal to 100%, 75% and 50% of the total fortnightly pan evaporation from the past 14 days were applied every fortnight as irrigation. These simulations will be called IPF100ET, IPF75ET and IPF50ET, where IP stands for irrigation practice, F represents a fortnightly irrigation interval, and 100ET indicates the percent of total fortnightly pan evaporation applied as irrigation. In the other three simulations, the irrigation interval was changed from 14 days to 7 days during the second half of the growing season. Weekly irrigation application amounts equal to 100%, 75% and 50% of the total weekly pan evaporation from the past 7

days were applied every week as irrigation. These simulations will be called IPM100ET, IPM75ET and IPM50ET, where M indicates a mixed irrigation interval of 14 days during the first half of the growing season and 7 days during second half. The model simulation using the actual observed irrigation data was termed as CIP (current irrigation practice).

Total irrigation and rainfall application was largest under CIP and lowest under IPF50ET (Figure 10). The ET was maximum under IPF100ET and lowest under IPF50ET. The total amount of water used as ET in the IPF100ET (825 mm) and IPF75ET (771 mm) was significantly higher than CIP (740). The maximum ET will therefore be likely if IPF100ET is adopted as irrigation practice. In fact, both IPF100ET and IPF75ET seem attractive with respect to total ET. The runoff and drainage losses were highest under CIP and lowest under IPF50ET (Figure 10). The total water lost as runoff under IPF100ET (255 mm) was significantly lower than that under CIP (640 mm). It was much lower for both IPF75ET and IP50ET than CIP. The same was true for the total amount lost to drainage (Figure 10). Most of the extra water applied as irrigation under CIP was either lost as runoff or drainage. In addition to evaluation of the distribution of total applied irrigation water into ET, runoff and drainage the availability of soil moisture between irrigations and the impacts on soil salinity were also assessed to enable the selection of an optimal irrigation strategy.



Figure 10. Water balances for the simulated irrigation options at KRS 7A; proportions of total applied irrigation water, ET, runoff and drainage.

The soil moisture profiles for CIP, IPF100ET, IPF75ET and IPF50ET, shown in Figure 11, represent the soil moisture content on the day before each irrigation date for seven irrigation events of the maize crop. The soil moisture content on the day before irrigation for the remaining four irrigation events, not shown in Figure 11, was above allowable depletion (AD). The wilting point and allowable depletion water content profiles also are shown in this Figure. The allowable depletion water content was assumed to be 0.5 of the total available water between field capacity and wilting point. The predicted soil moisture profiles for all irrigation strategies and monitoring dates always remained above the wilting point. Under CIP, the soil moisture content was less than the allowable depletion on September 15, 2004 and September 30, 2004 (Figure 11). For IPF100ET, there were three occasions when soil moisture in middle parts of the soil profiles was less than the AD. For IPF75ET and IPF50ET there were four and five occasions, respectively, when the soil moisture profiles were lower than AD (Figure 11). The soil moisture content was always above AD during first half of the growing season because of relatively small ET demand.

The soil moisture profiles of CIP were similar to IPF100ET with respect to the water availability for the crop. If it is assumed that the maize crop was already mature during the month of September and ready for harvest (no irrigation was applied during this month in CIP) then the impact of the last two soil moisture profiles on the crop water availability can be ignored; both of these were less than the AD. Accordingly, the CIP may appear to be the best irrigation practice with respect to soil water availability but, as discussed earlier, it caused the largest amount of wastage in the form of runoff and drainage. The predicted amount of water used as ET in the CIP also was less than that in the IPF100ET. The IPF100ET is therefore a better strategy with respect to both crop water availability and water saving. It would require around 11 ML/ha and deliver a net saving of 330 mm (23%) over one growing season without any significant crop water stress. The predicted water savings are likely to be achieved from reductions in the runoff and drainage. The IPF75ET would require around 8.4 ML/ha and deliver a net saving of around 40%; however, the crop would be under minor stress for a few days. This water requirement of 8.4 ML/ha is slightly higher than 7.5 ML/ha determined by [44] for the same crop in semi-arid tropical environments of Northern Territory (Katherine, Douglas Daly, Dalywaters, Mataranka, and Larrimah), Western Australia (Kununurra, Derby, and Broome) and Queensland (Gordonvale). In IPM75ET the level of stress was reduced by decreasing the irrigation interval from fortnightly to weekly in last half of the growing season (Figure 12). This resulted in wetter soil profiles than those under the IPF75ET during second half of the growing season. There was no significant build up of soil salinity and differences in the predicted soil salinity profiles over time among the various irrigation strategies.

It is important to maintain water availability above AD level especially during vegetative growth, flowering and reproductive stage of the maize crop because of its sensitivity to both water deficit and its timing. A significant reduction in yield can occur due to water deficit during both vegetative and reproductive period [37]. Both [37] and [38] conclude that the water deficit during flowering stage in particular has a devastating effect on maize yield. The IPM75ET irrigation strategy maintains favourable soil moisture conditions or water availability throughout the growing season thus saving water as well as ensuring an optimal yield.

Based on the above model predictions, it is concluded that irrigation application equal to 100% of total fortnightly pan evaporation at 14 days interval is a better irrigation strategy (IPF100ET) and would save around 23% water. An irrigation application amount equal to 75% of total fortnightly and weekly pan evaporation at 14 day interval during the first half of the growing season and 7 day interval during the second half would be the best irrigation option (IPM75ET) if it is practicable to change the irrigation interval. This irrigation strategy would save around 40% water.

### 5.2.2. Irrigation Scheduling of Sugarcane Crop—Deep Watertable

The irrigation intervals and amounts used to irrigate sugarcane in the experimental block CUM 55 during 2004-05 were applied to simulate the current irrigation



Figure 11. Soil moisture profiles the day before irrigations for the Maize crop at KRS 7A: CIP (top left), IPF100ET (top right), IPF75ET (bot. left) and IPF50ET (bot. right).

practice (CIP). Five irrigation application strategies, in addition to the CIP, were simulated to determine an irrigation schedule that would produce the maximum soil moisture availability, minimum runoff and drainage, maximum ET, and minimum salinity accumulation in the soil profile.

The first irrigation strategy is IPF100ET as used for maize. The second irrigation strategy (IPF75-100ET) uses an irrigation amount equal to 75% of the total fortnightly ET from previous two weeks applied every fortnight for the first quarter of the growing season and 100% of total fortnightly ET applied during the rest of the growing season. In the third irrigation strategy (IPF50-100ET) the irrigation amounts were 50% of the total fortnightly ET during first quarter of the growing season and 100% during rest. In the fourth irrigation strategy (IPM50-100ET), an irrigation application amount equal to 50% of total fortnightly ET was applied every fortnight during first quarter of the growing season and 100% of total weekly ET was applied every 7 days during remainder of the growing season. The fifth irrigation strategy (IPM50-75ET) was the same as the fourth, except the irrigation amount was 75% of total weekly ET during the final three-quarters of the growing season.

The total irrigation and rainfall amount was smallest for IPM50-75ET, largest for IPF100ET, and was similar for IPF50-100ET and IPM50-100ET (**Figure 13**). The total ET was lowest under CIP and largest under IPF100ET. It was significantly larger in all irrigation strategies than CIP. Its variation between irrigation strategies was small (2375-2265 mm), except CIP. The model predicted the highest runoff under CIP and lowest



Figure 12. Soil moisture profiles the day before IPM75ET irrigations for the Maize crop at KRS 7A.



Figure 13. Water balances for the simulated irrigation options at CUM 55; total applied irrigation amount, ET, runoff and drainage.

under IPM50-75ET. The total drainage was largest under IPF100ET and lowest under IPM50-75ET. Considering total ET, runoff and drainage together, IPM50-100ET and IPM50-75ET gave the best results; both had comparable total ET and less runoff and drainage than CIP. Assessments of the soil moisture availability and salt accumulation in the root zone also are required to identify the best irrigation strategy.

The soil moisture profiles on the day before each irrigation for CIP (**Figure 14**) show that there were only few dates when the soil moisture was above the allowable depletion level indicating that the sugarcane crop was under soil moisture stress. On some dates, the soil moisture was very close to the wilting point, and it is expected that the crop experienced moisture stress at least during



Figure 14. Soil moisture profiles the day before CIP irrigations for the Sugarcane crop at CUM 55.

these days. A small total ET under CIP also indicates that the crop was under moisture stress at least some days during the growing season. Neither the irrigation amounts nor the irrigation intervals were appropriate. The irrigation amounts were large, which resulted in excessive runoff; and the irrigation intervals were too long, which resulted in soil moisture stress.

Soil moisture stress or water deficits have varying effects on sugarcane crop development, biomass accumulation and partitioning of biomass to millable stalk and sucrose, both during the season and at final harvest [39]. Water deficits during the tillering phase significantly affects leaf area, tillering and biomass accumulation but have relatively little effects on final yield. However water deficits, after the leaf area index is reached over 2, have more deleterious effects on final yield of total biomass, stalk biomass and stalk sucrose [39]. Therefore it is highly likely that the water deficit occurred during the growing season under CIP had significant impacts on final yield of sugarcane. The predicted soil moisture profiles for the IPF100ET, IPF75-100ET, IPF50-100ET, IMP50-75ET were below AD level on some dates. The soil moisture profiles for IPM50-100ET, shown in Figure 15, were always above the AD level, except one date. This irrigation strategy (IPM50-100ET) is recommended for the sugarcane crop grown on the Cununurra clay in the ORIA. This strategy ensures to maintain favourable soil moisture conditions throughout the growing season which is a prerequisite for the maximum crop productivity. A total of about 2200 mm of water will be required for irrigation where crops are irrigated after half the soil water supply is depleted. This amount equates to about



Figure 15. Soil water content profiles the day before IPM50-100ET irrigations for the Sugarcane crop at CUM 55; 13/04/04 (left) to 07/06/05 (right).

22 ML/ha. About 78% of the total applied water will be used as ET, 12% will be wasted as runoff, and around 10% will be lost to drainage. This water requirement of 22 ML/ha is close to lower end of the range (22.7 to 23.8 ML/ha) estimated by [40] using the APSIM-sugarcane model for the sugarcane crop grown over Cununurra clay in ORIA. According to [41] the observed and modelled water requirement of the sugarcane crop in the Burdekin Delta, located on the dry-tropical coastal strip in North Queensland, was 20.5 to 20.3 ML/ha which is only slightly lower than 22 ML/ha estimated in this study. This comparison shows findings from this study are similar to those by [40] and [41]. This also confirms the suitability of the LECHC for irrigation scheduling of crops with an added advantage of salinity modelling. The salinity modelling for IPM50-100ET suggested that there was salt accumulation over time in some parts of the soil profile however, the accumulation was well below the threshold (170 mS/m) that would affect sugarcane crop productivity.

### 5.2.3. Irrigation Scheduling of Sugarcane Crop—Non-Saline Shallow Watertables

The calibrated LEACHC model was used to assess the impacts of non-saline shallow watertables on irrigation water requirements, irrigation scheduling and soil salinity risks. Two shallow watertable depths (1 and 2 m) with EC of 50 mS/m were considered in the modelling. It was

assumed that a sugarcane crop grown on Cununurra clay was present throughout a total simulation period of three years. For each watertable depth, four simulations were conducted; IPF75ET, IPF50ET, IPW75ET and IPW50ET, where F indicates a fortnightly irrigation interval, as above, and W indicates a weekly irrigation interval. Thus, IPW75ET denotes that the irrigation interval was seven days and the irrigation application amount was 75% of total fortnightly pan evaporation (ET). One year (May 2004 to April 2005) of pan evaporation and temperature data, obtained from the KRS weather station, were repeated in the subsequent two years of simulation. The model predicted significant ET contributions from the two shallow watertables; the shallower the watertable the greater the groundwater contribution to ET for a particular irrigation strategy (Figure 16). The groundwater contribution was maximum (60% of the total ET) from a 1 m deep watertable for IPF50ET and was minimum (26% of total ET) from a 2 m watertable for IPW75ET. According to [43] a 1 m deep watertable in a sandy loam soil provided 65% of sugarcane ET in India which is similar to that estimated in this study under IPF50ET. The study by [42] concluded that nearly all ET requirements of the sugarcane crop grown on light medium and medium clay or sandy loam soil in Australia can be met from watertable if it is within 1 m of the soil surface. This study confirms the findings from other studies conducted in Australia [42] and elsewhere [43] and suggests that at least



Figure 16. Predicted groundwater contributions to total ET for Sugarcane crop grown over non-saline (50 mS/m) 1 and 2 m deep watertables.

60% of ET requirements of the sugarcane crop can be met from shallow watertables which is not only a substantial water saving but also helps control watertables.

The predicted average soil EC profiles for both watertable depths increased slightly over time (**Figure 17**). The variation in the predicted average EC profiles among the simulated irrigation strategies and between two watertable depths was small. Although the average soil profile EC increased during the simulation period from the initial levels it remained well below the threshold for any adverse impacts on the sugarcane crop.

Based on the simulated results, the IPF50ET irrigation

strategy is recommended for sugarcane crops for non-saline shallow watertables of one to two m depth. The model predicted that this irrigation strategy will result in the maximum irrigation water use efficiency because a greater proportion of shallow groundwater is used for ET requirements. The model also predicted that this irrigation strategy will cause the accumulation of salts in the root zone during the simulation period but well below the threshold for any adverse impacts on the crop yield.

### 5.2.4. Irrigation Scheduling of Sugarcane Crop—Saline Shallow Watertables

The same eight simulations, as above for the non-saline watertables, were conducted except that the shallow watertables were assumed saline. In the first four, a saline watertable with an EC of 200 mS/m was fixed at 1 m depth. In the second four, the watertable was fixed at 2 m depth with an EC of 300 mS/m. The initial average soil profile EC was around 55 mS/m.

There was no significant difference between groundwater contributions to ET for crops grown over saline and non-saline watertables. The soil moisture availability between irrigations was similar in all irrigation strategies and was always above the AD level. The use of saline groundwater for ET requirements resulted in salt accumulation in the soil profile and average EC of the soil profile increased significantly over time for all irrigation strategies and watertable depths. At both watertable depths the predicted average soil profile EC over time was largest (> 900 mS/m) for irrigation strategy IPF50ET (**Figure 18** and **19**). Low irrigation application caused



Figure 17. Predicted average soil profile EC for Sugarcane crop grown over a non-saline (50 mS/m) 1 m deep watertable.



Figure 18. Predicted average soil profile EC for Sugarcane crop grown over a saline (200 mS/m) 1 m deep watertable.



Figure 19. Predicted average soil profile EC for Sugarcane crop grown over a saline (300 mS/m) 2 m deep watertable.

withdrawal of more water from the watertable which resulted in the highest average soil profile EC over time. The lowest average soil profile EC (> 500 mS/m) resulted from IPW75ET at both watertable depths but it was well above the level tolerable by the sugarcane crop.

In summary, the modelling suggests that the soil profile salinity risk will be high if a saline watertable exists for long periods at or above 2 m depth which is consistent with an earlier finding by [8]. Over irrigations may reduce the build up of soil profile salinity through flushing but it will result in excessive accessions to the watertable causing groundwater to rise even further. The recommended management strategy for a saline shallow watertable is to lower its level below 2 m by artificial deep open or sub-surface drainage first and then apply regular leaching applications to flush excessive salts from the root zone area into the drainage system [8]. Without this intervention, it is likely that high evaporative demands, extended fallow periods and low irrigation application will cause excessive accumulation of salts in the soil profile.

### 5.3. Application of Recommended Irrigation Strategies

This study identified irrigation strategies that ensure efficient water use, optimal crop water availability and minimal salinity risks for the maize and sugarcane crops in the ORIA. The practical application and feasibility of the recommended irrigation strategies including irrigation intervals and their variation within a growing season were confirmed through discussions with the Ord Irrigation Cooperative and farming community. New irrigation areas are being developed under Ord Stage 2, adjacent to the existing Stage 1 irrigation area, where large areas are likely to be allocated for sugarcane. Because of similar climate, soil and other conditions, the irrigation strategies identified for the sugarcane crop in the Stage 1 area will be applicable to this crop to be grown in Stage 2 area. Also because the Ord Stage 2 is largely a closed groundwater flow system it will be even more important to control deep drainage in this area. Any deep drainage in excess of irrigation requirements is likely to cause a rise in groundwater levels and increase the risk of soil salinity development.

Water resource availability for irrigation of the existing and new irrigated areas in the Ord is not likely to be a major issue as enough water resource is expected to be available to meet the current and likely future water demands by the irrigation industry. The practical application of the preferred irrigation techniques is therefore less important with respect to water saving in the ORIA and more important for achieving an optimal yield and controlling or reducing deep drainage especially under Ord Stage 2 to avoid the development of shallow watertables and soil salinity. An inefficient irrigation strategy that allows excessive deep drainage in Ord Stage 2 in particular will necessitate the installation of subsurface drainage systems to control rising watertables if crop productivity is to be maintained. Such drainage installations, whether open deep drains or subsurface systems often require significant investments and have associated problems of safe disposal of drainage waters.

The irrigation water requirements assessed using LEACHC were compared with findings from other studies to test the applicability of the LEACHC model for irrigation scheduling and salinity management and extending the results to other regions in Australia. The water requirements assessed in this study were similar to those of the maize crop estimated by [44] at Kununurra (Ord), Derby and Broome in Western Australia; Katherine, Douglas Daly, Dalywaters, Mataranka, and Larrimah in Northern Territory; and Gordonvale in Queensland. This confirms both the applicability of these findings to other regions of Australia and the suitability of LEACHC for such a purpose. Similarly the sugarcane water requirements of 20.5 ML/ha to 23 ML/ha determined by [40] in the Ord and by [41] in the Burdekin Delta are similar to the water requirements of 22 ML/ha determined here. It means that the water requirements of

### 6. Conclusions

This study found that the irrigation application amounts equal to 100% of the total fortnightly pan evaporation, applied at 14 days interval, would be a better irrigation strategy for maize crop grown on Cununurra clay over a deep watertable. The predicted irrigation water use would be around 23% less than the exiting practice. Irrigation application amounts equal to 75% of the total fortnightly pan evaporation, applied every fortnight during first half of the growing season, and 75% of the total weekly pan evaporation, applied every week during the second half of the growing season, would be the best irrigation strategy if it is feasible to change the irrigation interval from 14 days to 7 days. The irrigation water use for this irrigation strategy was predicted to be around 40% less than the existing irrigation practice.

The study found that the best irrigation strategy for the sugarcane crop grown on Cununurra clay over a deep watertable would be irrigation application amounts equal to 50% of the total fortnightly pan evaporation, applied every fortnight during first quarter of the growing season, and irrigation application amounts equal to 100% of total weekly pan evaporation, applied every week during rest of the season. This irrigation strategy would require around 22 ML/ha of irrigation water for a single sugarcane crop.

The best irrigation strategy for the sugarcane crop grown over a non-saline shallow watertable of  $\leq 2$  m depth would be irrigation application amounts equal to 50% of the total bi-weekly pan evaporation, applied every 14 days. The model predicted that this irrigation strategy would result in the best water use efficiency by encouraging plants to use groundwater to meet the crop ET requirements. The modelling results indicated that the soil salinity risks would be high if the sugarcane crop was grown for long periods over a saline shallow watertable ( $\leq 2$  m). The best management strategy would be to lower the watertable below 2 m depth by artificial drainage first and then apply regular leaching applications to flush excessive salts into the drainage system.

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55

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56

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# **TABLE OF CONTENTS**

Volume 1 Number 1	September 2010
Sorption Characteristics of CO <sub>2</sub> on Rocks and Minerals in Stori	ng CO <sub>2</sub> Processes
T. Fujii, S. Nakagawa, Y. Sato, H. Inomata, T. Hashida	1
Evaluation of Various Linear Regression Methods for Downscal	ing of Mean Monthly
Precipitation in Arid Pichola Watershed	
M. K. Goyal, C. S. P. Ojha	11
Modeling of Asphaltene Grading in Oil Reservoirs	
J. Y. Zuo, O. C. Mullins, C. L. Dong, D. Zhang	
Combined Generalized Hubbert-Bass Model Approach to Inclu	de Disruptions When
Predicting Future Oil Production	
S. H. Mohr, G. M. Evans	
Modelling Irrigation and Salinity Management Strategies in the	e Ord Irrigation Area
R. Ali, J. Byrne, T. Slaven	

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Natural Resources. 2010, 1, 1-56.