Adding value to Marula: Modelling of the extraction of valuable compounds from *Sclerocarya birrea*

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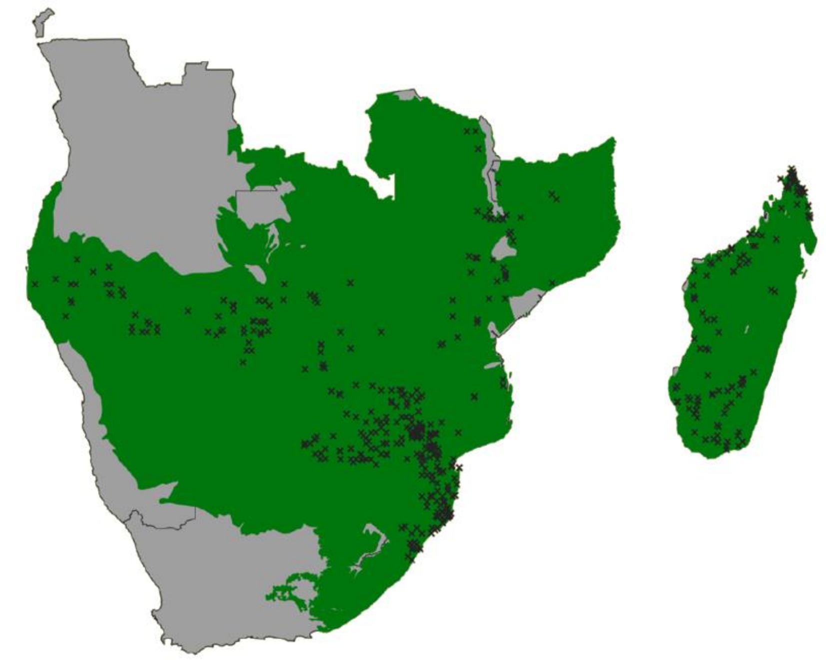
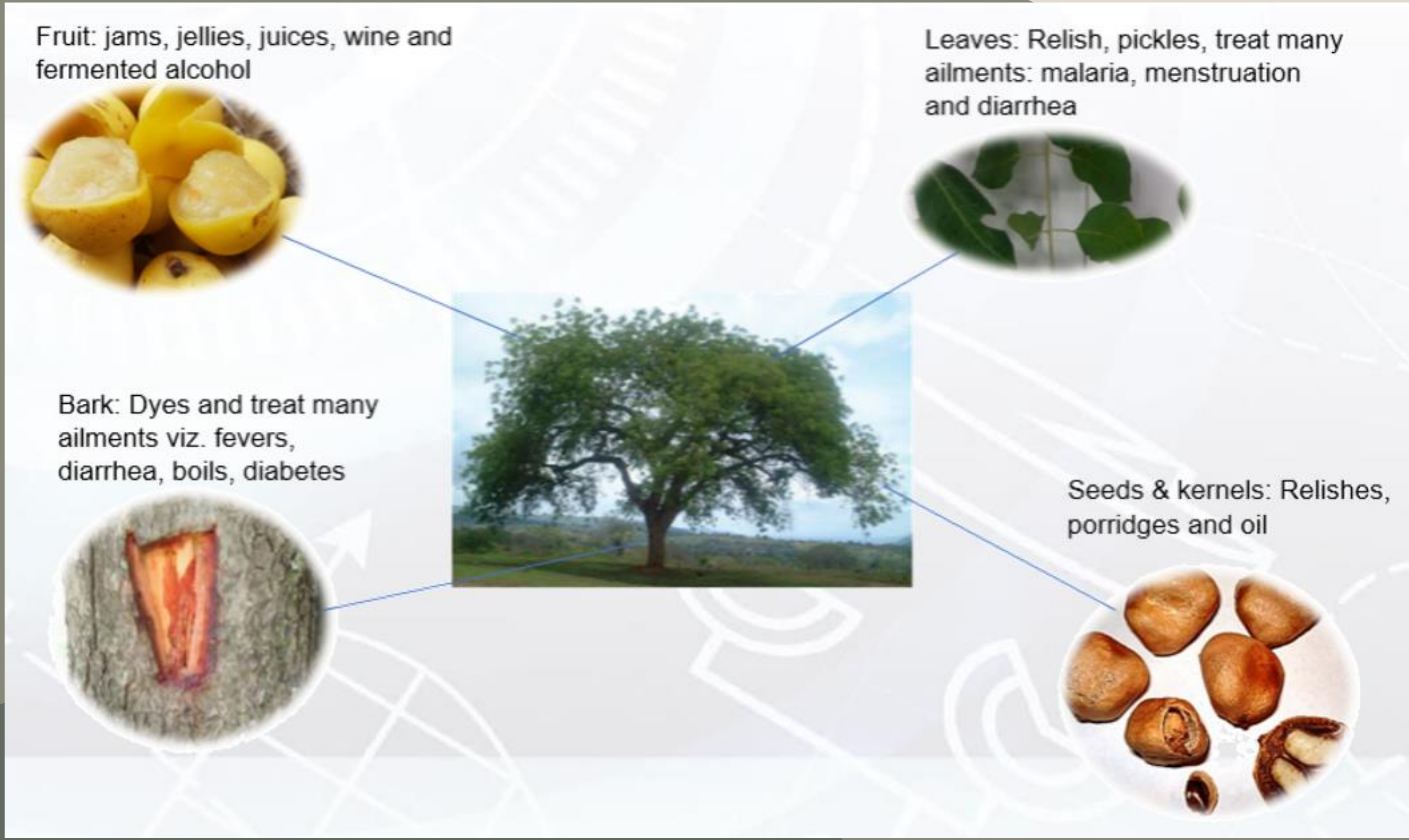
About marula:





Common names: marula (English); maroela (Afrikaans); morula (Tswana); and umGanu (isiZulu)

Problem Statement

No empirical studies or mathematical models have been developed on the extraction of marula oil.

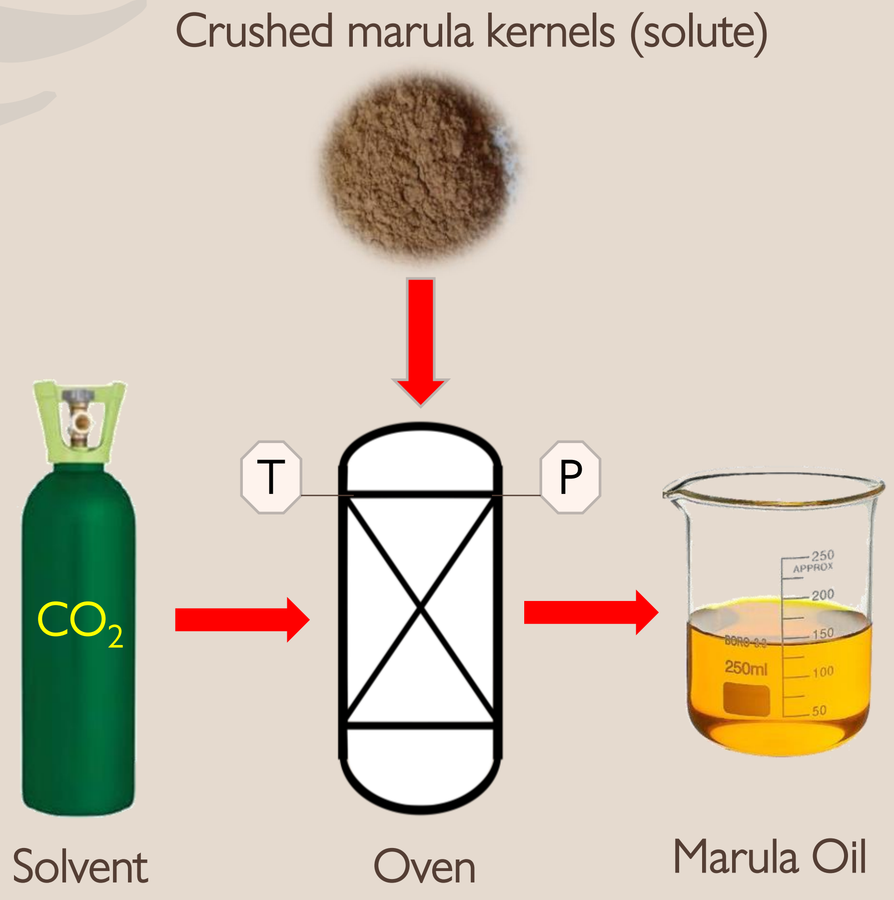
Aim

The aim of the study is to determine suitable mathematical and empirical models for the extraction of marula kernel oil.

Objectives

- Application of modelling to determine the yield of marula oil using experimental data of supercritical fluid extraction process from literature.
- Application of mathematical modelling to determine the oil yield of Sclerocarya birrea kernel oil using response surface methodology.

Supercritical Fluid Extraction Process



Experimental data from literature

Experimental run number	Temperature (°C)	Pressure (bar)	Observed Response (g oil/L CO_2)
1	40	250	5.808
2	60	250	3.542
3	75	250	1.851
4	40	350	8.135
5	60	350	7.853
6	75	350	7.757
7	40	450	8.483
8	60	450	9.221
9	75	450	8.93

Empirical Modelling

Model	Equation	Symbol definitions
Chrastil	$Y = \rho^k e^{\frac{A}{T}+B}$	Y = concentration of the solute in the solvent in g.L^{-1}
Del Valle & Aguilera	$Y = \rho^k e^{\frac{A}{T}+B+\frac{C}{T^2}}$	ρ is the density of the solvent in g.L^{-1}
Adachi & Lu	$Y = \rho^{(k+D\rho+E\rho^2)} e^{\frac{A}{T}+B}$	T is the temperature of the solvent in Kelvin
Sparks et al.,	$Y = \rho^{(k+D\rho+E\rho^2)} e^{\frac{A}{T}+B+\frac{C}{T^2}}$	k, A, B, C, D and E are model constants that can be determined by manipulating the experimental data.
Kumar & Johnston	$\ln(y_2) = \frac{A}{T} + B + C\rho$	Y_2 is the mole fraction of the solute in the solvent.
Méndez-Santiago & Teja	$\ln(Py_2) = \frac{A}{T} + B + C\frac{\rho}{T}$	P is the operating pressure in mPa

Mathematical Modelling

$$Y = \partial_O + \sum_{i=1}^{n} \partial_i x_i + \sum_{i=1}^{n} \partial_{ii} {x_i}^2 + \sum_{i=1}^{n} \sum_{j=i+1}^{n} \partial_{ij} x_i x_j$$

Where:

Y represents the response or dependant variable.

∂_O is a constant.

∂_i are the coefficients of the linear terms.

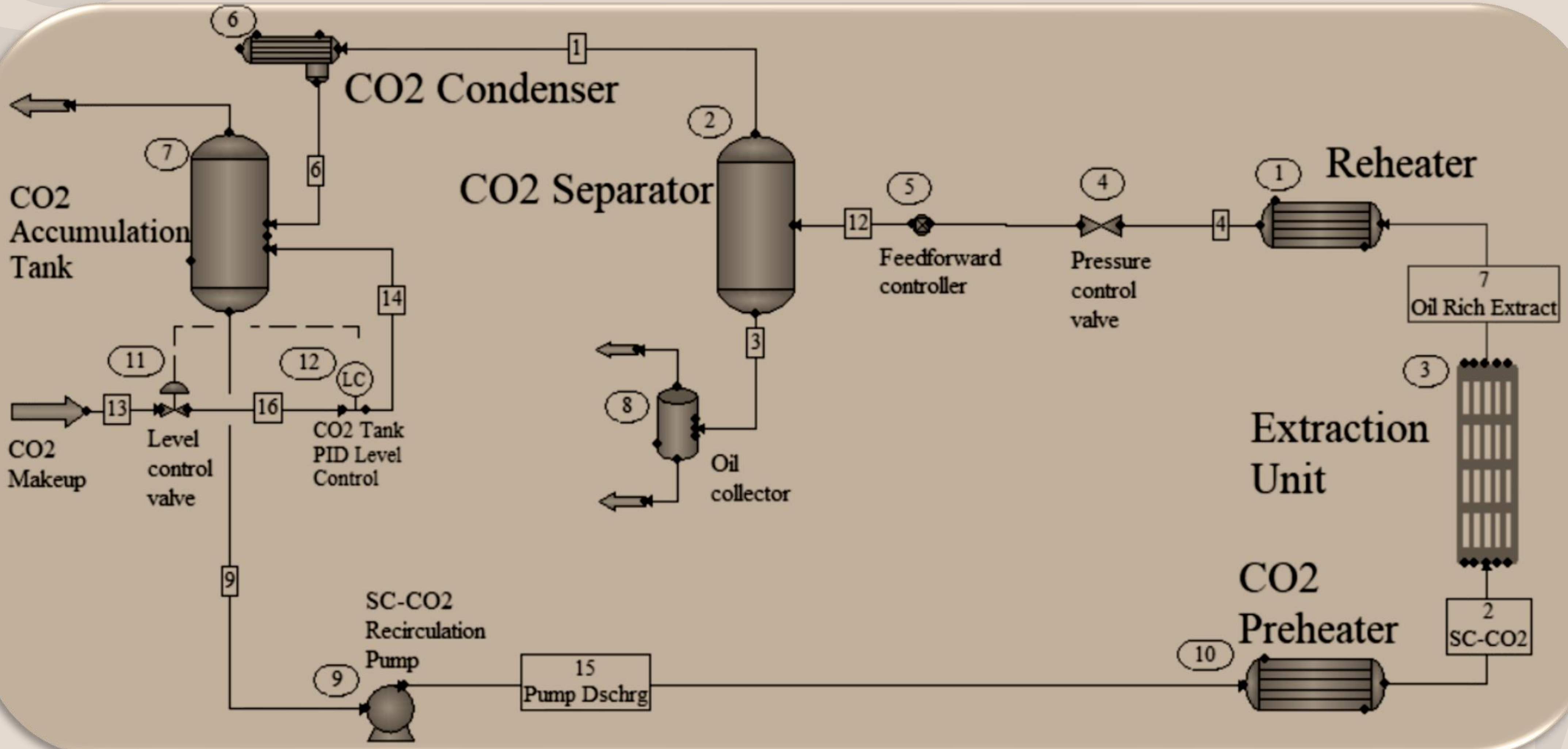
∂_{ii} are the coefficients of the quadratic terms.

∂_{ij} are the interactive coefficients.

x_i and x_j represents the independent variables.

n is the index of summation.

The importance of modelling



Results: Empirical Modelling

Model	Equation	Modelled equation	Determination coefficient (R^2)	Average absolute relative deviation (AARD%)
Chrastil	$Y = \rho^k e^{\frac{A}{T}+B}$	$Y = \rho^{5.33} e^{\frac{-1960}{T}-28.18}$	0.87	7.94
Del Valle & Aguilera	$Y = \rho^k e^{\frac{A}{T}+B+\frac{C}{T^2}}$	$Y = \rho^{5.33} e^{\frac{-1967.57}{T}-28.20+\frac{0.0000813}{T^2}}$	0.87	7.92
Adachi & Lu	$Y = \rho^{(k+D\rho+E\rho^2)} e^{\frac{A}{T}+B}$	$Y = \rho^{(5.33+0.00025\rho-0.00000031\rho^2)} e^{\frac{-2013}{T}-27.90}$	0.75	14.90
Sparks et al.,	$Y = \rho^{(k+D\rho+E\rho^2)} e^{\frac{A}{T}+B+\frac{C}{T^2}}$	$Y = \rho^{(5.33-0.0005\rho+0.000000450\rho^2)} e^{\frac{-2023}{T}-27.59+\frac{-2516}{T^2}}$	0.72	15.53
Kumar & Johnston	$\ln(y_2) = \frac{A}{T} + B + C\rho$	$\ln(y_2) = \frac{-1587.63}{T} - 7.57 + 0.0051\rho$	0.94	5.12
Méndez-Santiago & Teja	$\ln(Py_2) = \frac{A}{T} + B + C\frac{\rho}{T}$	$\ln(Py_2) = \frac{-6652.35}{T} + 6.80 + 3.37\frac{\rho}{T}$	0.95	0.049

High R^2 = ☺

Low R^2 = ☹

Low AARD% = ☺

High AARD% = ☹

Results: Empirical Modelling

				Predicted values (g oil/L CO_2)			
Temperature (°C)	Pressure (bar)	Density (g/L)	Experimental values (g oil/L CO_2)	Chrastil	DVA	AL	Sparks et al.,
40	250	880	5.808	5.376	5.3694	5.384	5.053
60	250	787	3.542	4.317	4.3153	5.157	3.487
75	250	712	1.851	3.262	3.2624	4.354	2.429
40	350	935	8.135	7.426	7.4193	6.609	7.921
60	350	863	7.853	7.055	7.0560	7.380	6.502
75	350	808	7.757	6.401	6.4051	7.442	5.395
40	450	975	8.483	9.283	9.2768	7.512	11.002
60	450	913	9.221	9.525	9.5284	8.993	9.780
75	450	867	8.930	9.3177	9.3278	9.738	8.743

Results: Empirical Modelling

				Predicted values (Mole fraction)	
Temperature (°C)	Pressure (bar)	Density (g/L)	Experimental values (Mole fraction)	Kumar and Johnston	Méndez-Santiago and Teja
40	250	880	0.000283	0.000281	0.000276
60	250	787	0.000220	0.000238	0.000218
75	250	712	0.000127	0.000199	0.000177
40	350	935	0.000397	0.000372	0.000356
60	350	863	0.000383	0.000350	0.000336
75	350	808	0.000379	0.000325	0.000321
40	450	975	0.000414	0.000455	0.000426
60	450	913	0.000450	0.000451	0.000434
75	450	867	0.000436	0.000438	0.000441

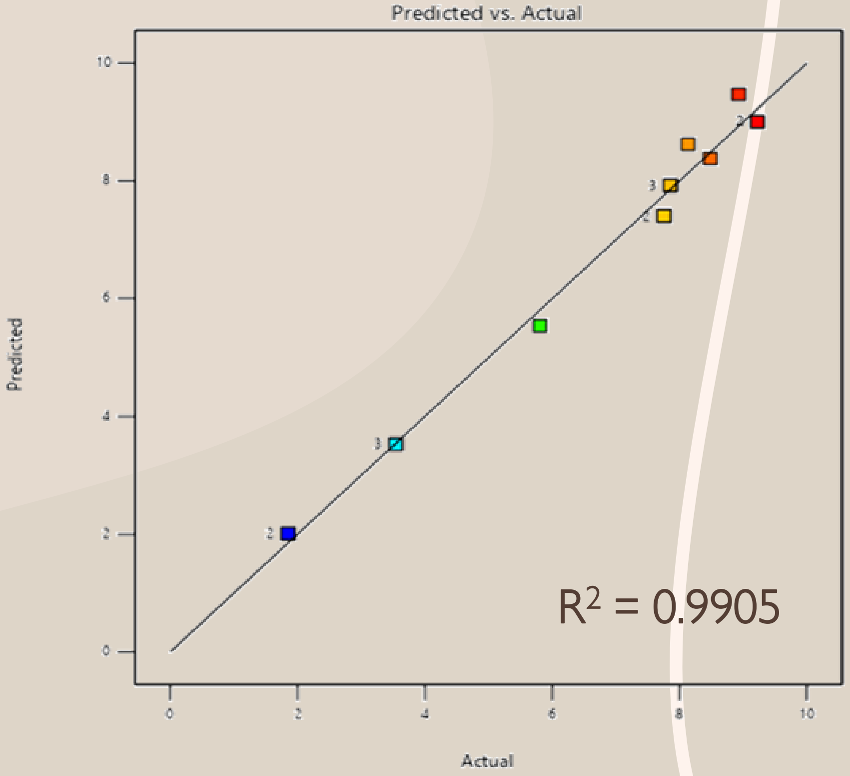
Results: Mathematical modelling

The second-order polynomial equation was used to express the solubility of marula kernel oil in supercritical carbon dioxide:

$$Oil\ Yield\left(\frac{g\ oil}{L\ CO_2}\right) = -6.89065 - 0.238031T + 0.104401P + 0.000657TP - 0.000230T^2 - 0.000166P^2$$

Where: T = Temperature in °C, P = Pressure in bar

Experimental run number	Temperature (°C)	Pressure (bar)	Observed response (g oil/L CO_2)	Predicted response (g oil/L CO_2)
1	40	250	5.808	5.515
2	60	250	3.5415	3.580
3	75	250	1.8512	2.007
4	40	350	8.1345	8.623
5	60	350	7.8533	8.002
6	75	350	7.7568	7.415
7	40	450	8.4825	8.412
8	60	450	9.2213	9.104
9	75	450	8.9301	9.502



Thank you

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