"Computational Assignment"

By Amit Kumar
(200109)

SYSTEM - "Water (1) and Morpholine (2)"

Activity Coefficient Model - Margules

$$A_{12} = 0.1776 \qquad A_{21} = -0.219$$

$$\ln \gamma_1 = [A_{12} + 2(A_{21} - A_{12})x_1]x_2^2$$
$$= [0.1776 + 2(-0.1776 + 0.219)x_1]x_2^2$$
$$= [0.1776 + 0.7932 x_1]x_2^2$$

$$\ln \gamma_2 = [A_{21} + 2(A_{12} - A_{21})x_2]x_1^2$$
$$= [-0.219 + 2(0.1776 + 0.219)x_2]x_1^2$$
$$= [-0.219 + 0.7932 x_2]x_1^2$$

here Pressure is Const. $P = 563.00$ mm Hg.

In Antoine eqn. use P ~~as~~ P^{sat} to get some initial value of T^{sat}

$$T_i^{sat} = \frac{B_i}{A_i - \ln P} - C_i \quad \rightarrow T_1^{sat}, T_2^{sat}$$

⇒ "I ~~take~~ took 101 values of x_1 from 0 to 1 with ~~0.01~~ adition of 0.01"

$x_1 = 0, 0.01, 0.02, 0.03, \ldots 0.98, 0.99, 1.00$

⇒ Let's move ahead with any x_1

Take weighted average to get intial T:

$$T = T_1^{sat}(x_1) + T_2^{sat}(x_2)$$
$$\hookrightarrow x_2 = 1 - x_1$$

Next Calculate P_1^{sat}, P_2^{sat} By Antoine eqn

$$\ln P^{sat} = A - \frac{B}{T+C}$$

Define a α such that

$$\alpha = \frac{P_1^{sat}}{P_2^{sat}}$$

→ modified Roult's law

$$P = x_1 \gamma_1 P_1^{sat} + x_2 \gamma_2 P_2^{sat}$$

$$(P)(P_1^{sat}) = (x_1 \gamma_1 P_1^{sat} + x_2 \gamma_2 P_2^{sat})(P_1^{sat})$$

$$P_1^{sat} = \frac{P(P_1^{sat})}{x_1 \gamma_1 P_1^{sat} + x_2 \gamma_2 P_2^{sat}}$$

$$\boxed{P_1^{sat} = \frac{P}{x_1 \gamma_1 + \frac{x_2 \gamma_2}{\alpha}}}$$

Calculate P_1^{sat} from here

T = calc. new value of T using Antoin eqn

$$T = \frac{B}{A - \ln P_1^{sat}} - C$$

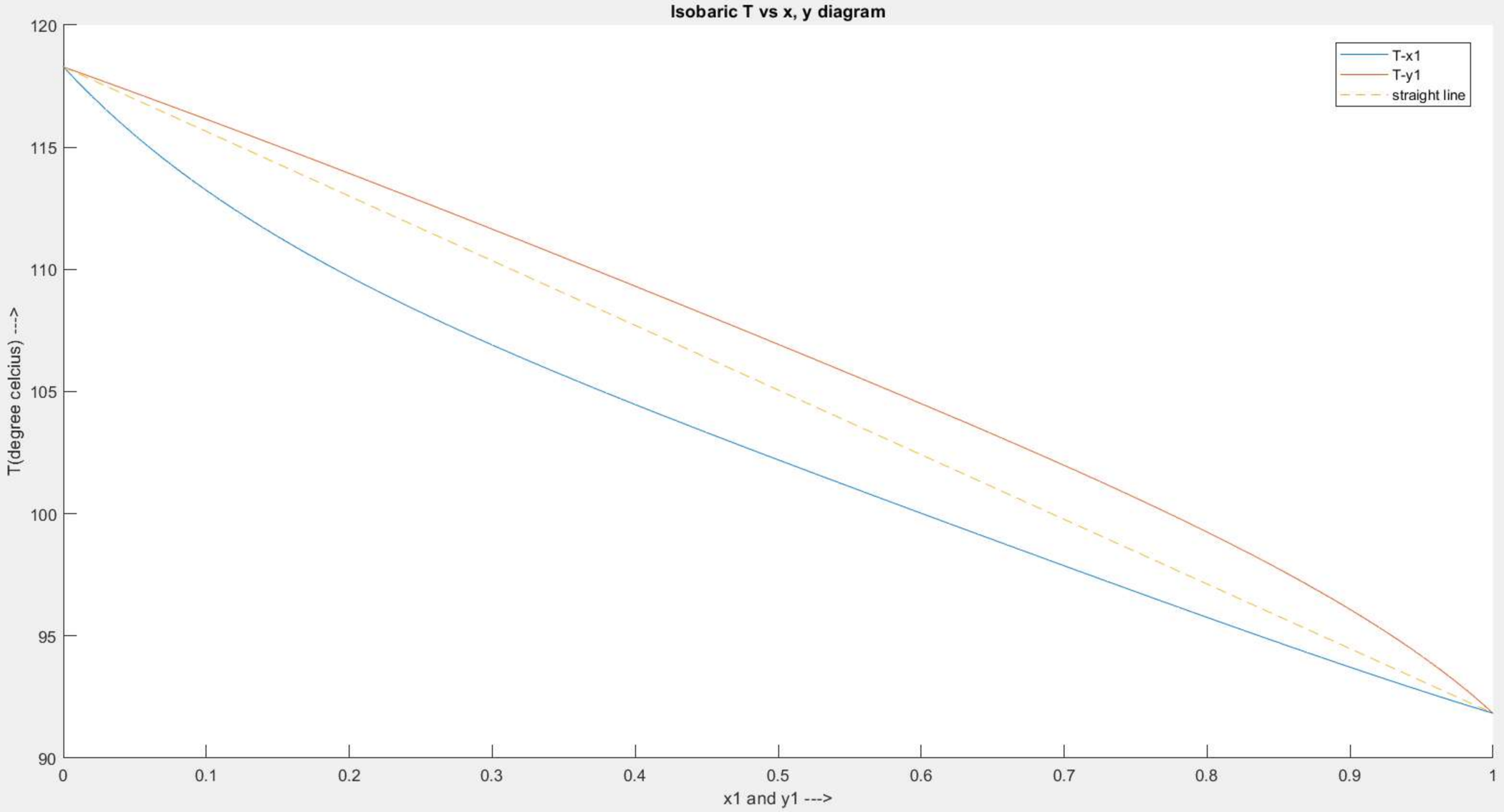
Now Reapet this process untill convergence

And then calc. $y_1 = \frac{x_1 \gamma_1 P_1^{sat}}{P}$

⇒ Do this ~~whole~~ whole process for each value of x_1 (0, 0.01, 0.02 - - -) and plot them on graph with T.

Figure 1

File Edit View Insert Tools Desktop Window Help

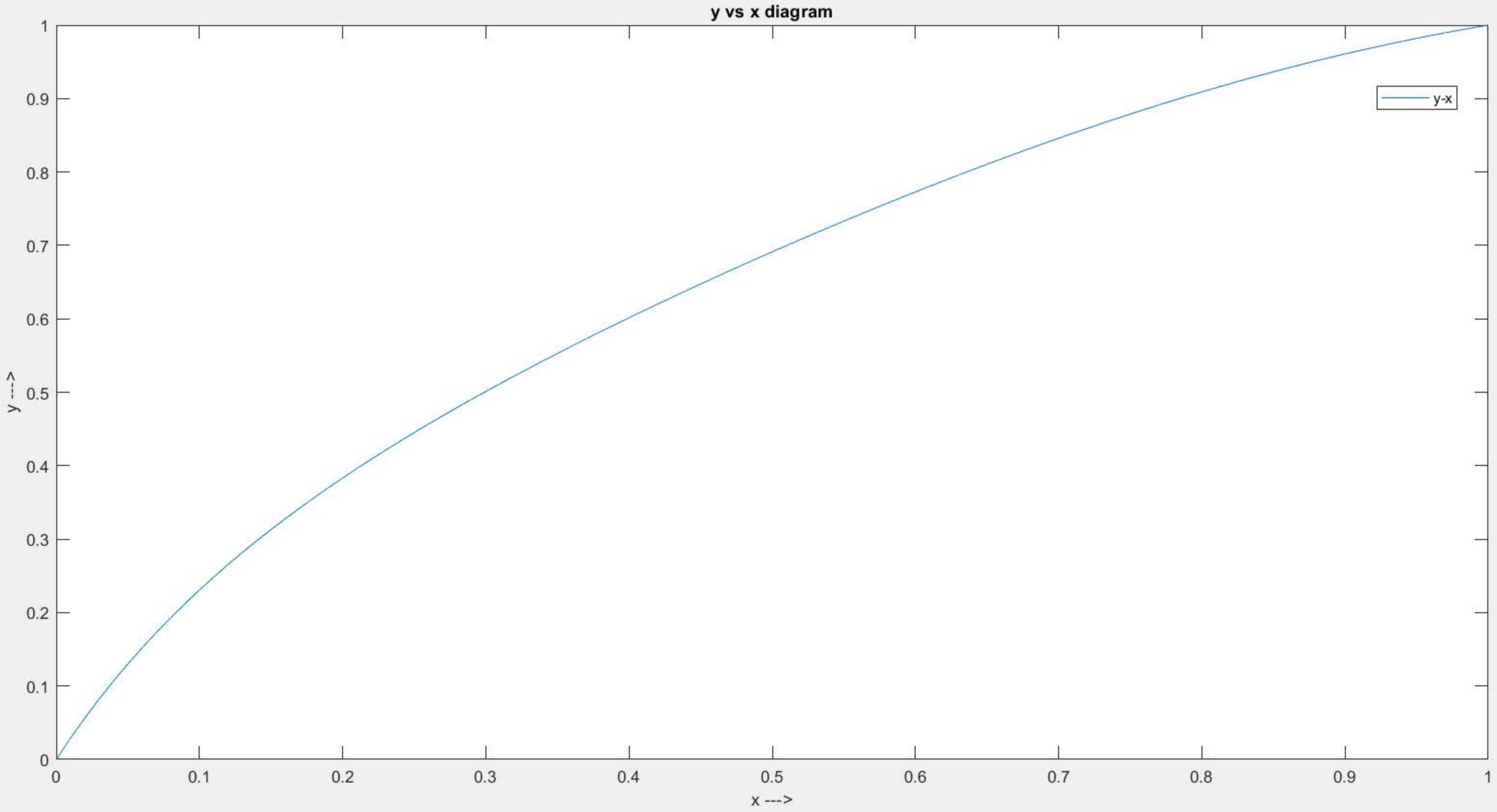


Type here to search

4:34 PM
09-Apr-22

Figure 2

File Edit View Insert Tools Desktop Window Help

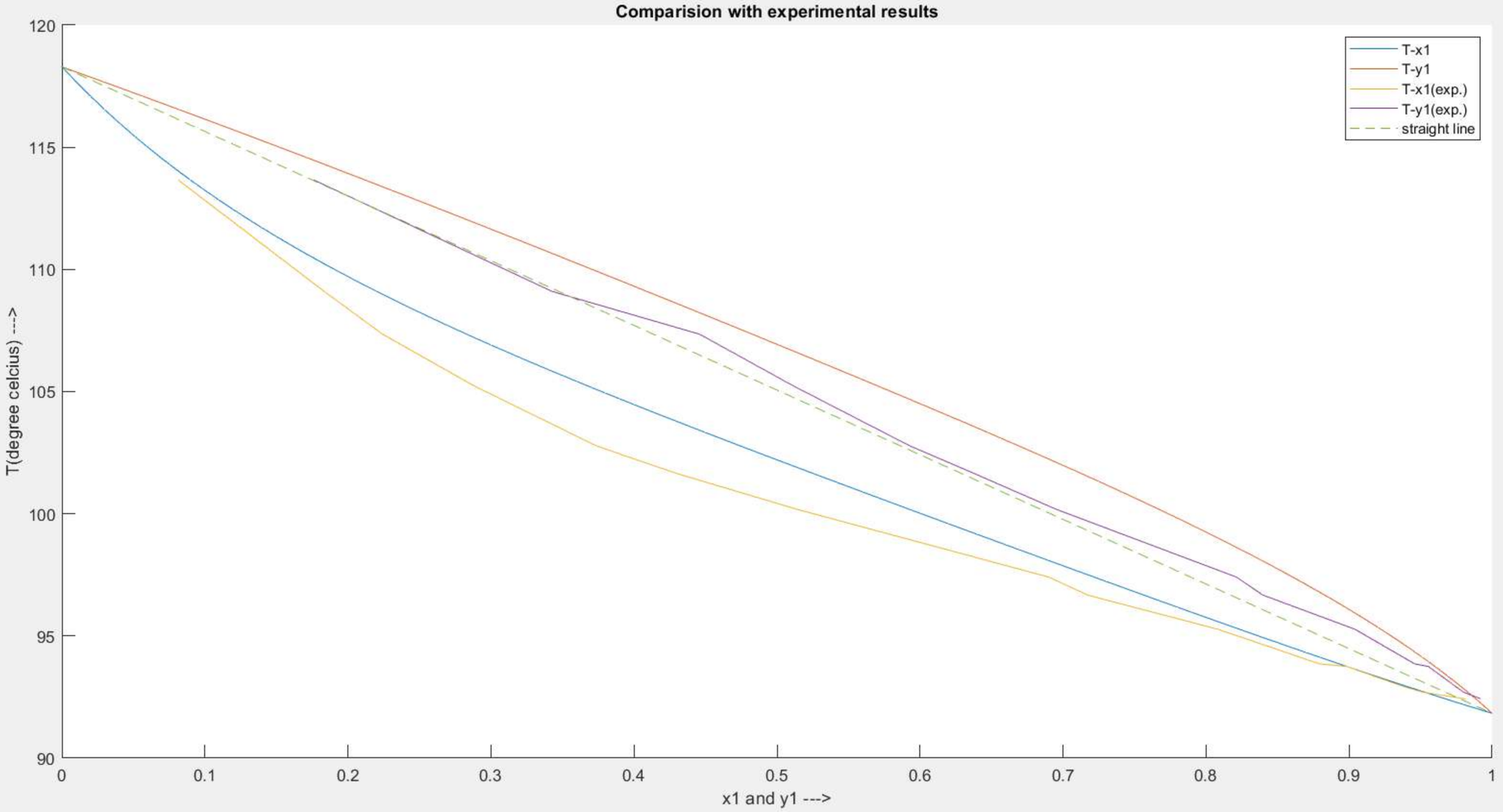


Type here to search

4:33 PM
09-Apr-22

Figure 3

File Edit View Insert Tools Desktop Window Help



Type here to search

4:33 PM
09-Apr-22