Studies on the Continuous Inversion of Sucrose:
II, Application of Research Data

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Received for publication May 25, 1972

During its twenty plus years' history, the commercial production of invert syrups has generated large quantities of information. Of this information, very little was applicable to the production of invert syrups in a continuous process.

With the decision made to develop and install a continuous invert syrup production facility, the Engineering design group was faced with a series of questions which could not be answered from known operating experience. Such items as: (a) Specification as to the type and size of a continuous reactor; (b) Specification of and permissible variation in the critical control loops; and (c) Establishment of the various operating parameters would have to be obtained before a firm design was undertaken. The development of a mathematical model of the inversion of sucrose permitted us to fix the many unknowns, and develop the design for a successful continuous invert group syrup production facility.

Basically, the production of invert syrup is an application of the acid catalyzed hydrolysis of sucrose for which time, temperature and acid concentrations are the principal variables. From chemical reaction kinetics we may write the following three reaction rate equations:

$$(1) \quad \frac{dC_s}{dt} = - kC_sC_wC_H$$

$$(2) \quad \frac{dC_w}{dt} = - kC_sC_wC_H$$

$$(3) \quad \frac{dC_i}{dt} = - 2\ k\ C_sC_wC_H$$

In these equations C_s, C_w and C_H represent the concentrations of sucrose, water, hydrogen ion, and invert. All concentrations are in English engineering units of pound moles per cubic foot and time

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in minutes. These equations express the quantitative relationships between the concentration of each of the chemical species, time, and the specific reaction rate or velocity constant "k." Provided sufficient data are available, the velocity constant "k" can be evaluated.

Our research department was requested to determine the time required to produce invert syrup at three different acid concentrations and at three different temperatures. Because of control difficulties on small bench scale experiments, 51% inversion of available sucrose was achieved. The following table summarizes these data:

Table 1.—Time required to invert 51% of available sucrose.

	Acid concentration, lb moles/ft		
Temperature °C	1.66×10^{-4}	2.14×10^{-4}	2.59×10^{-4}
85	19.2 min	12.2 min	9.4 min
90	12.3	7.8	5.8
100	4.1	2.7	2.2

The data as plotted in Figure 1 show some slight inconsistencies. According to theory, a family of parallel straight lines should have been obtained. Therefore, it was necessary to slightly bias the curve fitting to the data so as to achieve a uniform fit. Using plotted values for the time rather than the actual determined values, the specific reaction rate constant was estimated by considering the reaction to be 2nd order with the concentration of hydrogen ion being held constant. Values were as follows:

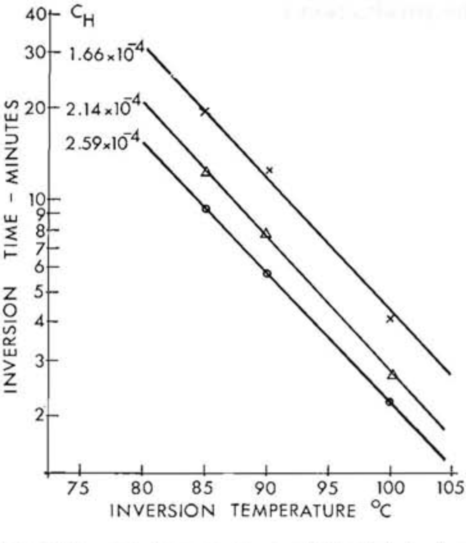

Figure 1.—Inversion vs. temperature plot of data from Table 1.

Table 2.—Estimation of velocity constant (basis 2nd order reaction rate).

	Acid concentration - lb moles/ft^3		
Temperature °C	1.66×10^{-4}	2.14×10^{-4}	2.59×10^{-4}
85	0.038	0.061	0.078
90	0.063	0.101	0.128
100	0.170	0.268	0.335

As the hydrogen ion concentration remains constant during an acid catalyzed reaction, each of the above velocity values may then be converted to its 3rd order reaction constant by dividing by the hydrogen ion concentration.

Table 3.—Estimation of velocity constant (basis 3rd order reaction rate).

	Acid Concentration - lb. moles/ft^3		
Temperature °C	1.66×10^{-4}	2.14×10^{-4}	2.59×10^{-4}
85	228	285	301
90	378	472	494
100	1020	1252	1293

From the Theory of Reaction Rates, the following quantitative relationship is given:

$$k = A_f \, e^{-\frac{Ha}{RT}} \tag{4}$$

where
A_f = A frequency factor
e = Base of natural logs
Ha = Activation energy BTU/lb mole
R = Universal gas constant
T = Absolute temperature, °R

Evaluation of A_f and H from the above data yielded the following average values.

$$A_f = 3.5 \times 10^{18}$$
$$Ha = 45{,}200 \text{ BTU/lb mole}$$

The use of these values in an analog computer program was awkward and presented difficulties due to the multiplication of an extremely large number by an extremely small one (i.e., $e^{-\frac{Ha}{RT}}$ has a magnitude of 10^{-16}). From a plot of the velocity constant values at various temperatures and acid concentrations, it should be possible to derive a similar expression in terms of only temperature and acid concentrations, which would yield comparable values. Utilizing a statistical approach it was found that:

a) A_f could be replaced by a constant (73.9) multiplied by the hydrogen ion concentration.

b) The value of $\frac{Ha}{RT}$ could be replaced by the expression (0.0550 $-10 \times C_H$) T where T is in degrees Fahrenheit.

The above substitution is in agreement with theory in that a generalized acid-base catalyzed homogeneous reaction, the concentration of the catalyst affects both the activation energy and frequency factor.

The inversion of sucrose is an exothermic reaction. During the course of the reaction, heat is liberated which raises the process temperature and thereby increases the rate of reaction. Thus, the temperature rise in a reacting sucrose solution is proportional to the amount of sucrose reacted, and is independent of the total amount of syrup present. We may then state that:

$$T = To + \frac{E}{WC_p} kC_sC_wC_H \tag{5}$$

where: T = Reaction temperature
To = Initial temperature
E = Heat of reaction
Cp = Specific heat
W = Weight per cubic foot

The combination of the five equations constitutes a mathematical description of the invert process. When programmed into an analog computer, it was possible to follow the decrease in sucrose concentration as a function of time for any given set of initial conditions. Typical results are shown plotted in Figure 2.

Working with similar plots for other initial conditions, we were able to specify a minimum size reactor which would yield the design throughputs. We could then size and specify the feed rate (time), acid metering rate, and reactor input temperature. Application of "sensitivity analysis" to the formula permitted us to specify the necessary instrument control accuracy.

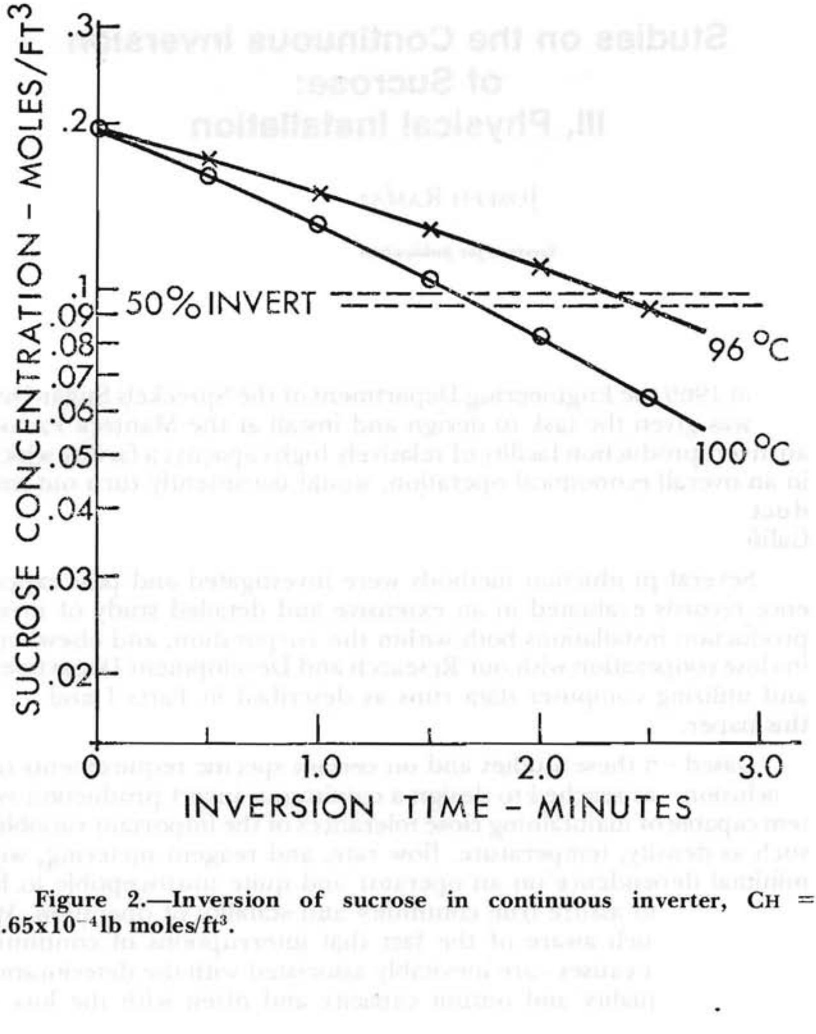

Figure 2.—Inversion of sucrose in continuous inverter, $C_H = 2.65 \times 10^{-4}$ lb moles/ft^3.