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Modelling of ethanol evaporative losses during batch alcohol fermentation

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Abstract

A general theoretical model to predict evaporative ethanol losses during the industrial process of batch alcohol production by fermentation is suggested. The model takes into account the combined effects of several yield loss factors. It also includes kinetic equations to predict product formation as a basis for calculating evaporative rates.

The model has been compared with others reported in the literature and a compilation of experimental data from different discontinuous processes has been used for verification, at both industrial and laboratory levels. The results show the suggested model to yield higher theoretical consistency as well as better adaptability to actual experimental data.

1. Introduction

Volatile product evaporation during batch processing is one of the main reasons for losses in industrial alcohol fermentations. High capacity discontinuous equipment (10 000–200 000 l) is characteristic of the fermentation alcohol industry because of the seasonal and decaying nature of the raw materials. Under these conditions, a large amount of gas saturated with volatile compounds is released from the fermenter. This constitutes a major yield loss in the case of ethanol. Ethanol losses from evaporation in industrial fermentations are estimated to be from 1% to 3% of the ethanol produced [1], and these losses are estimated to be from 10% to 30% of the total observed yield losses [2].

The development of accurate kinetic models for industrial alcohol fermentation demands that all the factors influencing the obtained alcohol yield must be taken into account; like product evaporation, substrate metabolism via respiration or secondary compound formation (glycerol, amino acids, etc.). It is also necessary to know the influence of several variables, e.g. temperature, on each of these factors.

To date, few models for industrial alcohol fermentation have taken evaporation into account [3, 4]. Even in these cases, the influence of media composition or the combined effect of different yield loss factors has been neglected. In this paper, a general evaporation model including the most important variables relating to the phenomenon is suggested.

2. Evaporation model

Evaporation can be assumed to be exclusively controlled by the thermodynamic equilibrium established between the gas bubbles and the liquid phase itself. The bubbles are generated by the microorganisms inside the fermentation environment and the liquid phase is the fermenting medium. This assumed equilibrium is reasonable owing to the normally small size of the bubbles (1–3 mm diameter); and owing to the negligible mechanical drag of liquid on the gas flow [5–7].

In addition, the gas phase is assumed to be made up exclusively from the major volatile compounds: carbon dioxide (c), water (w) and ethanol (e). Partial pressure additivity is also assumed. In this way, the gas composition can be represented by the following system of equations

$$
\begin{aligned}
&p = p_c + p_w + p_e \\
&y_e = \frac{p_e}{p} \\
&y_w = \frac{p_w}{p} \\
&y_c = 1 - y_e - y_w
\end{aligned}
\qquad (1)
$$

where p is the total gas pressure in the gas flow (usually atmospheric pressure); p_i is the partial pressure of compound i; and y_i is the molar fraction of compound i in the gas phase.

Owing to the fermentation liquid phase not being an ideal system, the following equilibrium equation is applied

$$p_i = p_i^0 \gamma_i x_i \qquad (2)$$

where p_i^0 is the vapour pressure of pure component i; γ_i is the activity coefficient of component i; and x_i is the molar fraction of compound i in the liquid phase (this can be obtained either experimentally or from kinetic equations).

To calculate p_i^0 according to the temperature of the fermentation environment, Antoine's equation can be used

$$\ln p_i^0 = A_i - \frac{B_i}{T - C_i} \qquad (3)$$

where A_i, B_i, and C_i are the corresponding Antoine coefficients for each compound ($A_e = 18.9119$; $B_e = 3803.98$; and $C_e = 41.68$, for pressure in millimetres of mercury and temperature in kelvins).

As for the activity coefficients, owing to the high water ratio in the liquid phase, $\gamma_w = 1$ can be considered reasonable. On the other hand, γ_e is a function of temperature, ethanol concentration in the liquid and type and concentration of dissolved compounds. There are several theoretical methods for determining the ethanol activity coefficient in multicompound mixtures [8, 9]; nevertheless, the results are too involved for complex cases such as natural fermentation media. Furthermore, there are no data available for some of the necessary parameters of the system components. Instead, empirical equations which show good results under the usual working conditions can be used.

The first thing to calculate is the ethanol activity coefficient for the ethanol–water pure binary mixture (γ_e^0), using the following equation [10]

$$
\begin{aligned}
&\ln \gamma_e^0 = A - \frac{B}{T} \frac{T - T_\gamma^0}{T_\gamma^0} \\
&A = a_1 e^{-a_2 x_e} \\
&B = b_1 - b_2 X_e
\end{aligned}
\qquad (4)
$$

where $T_\gamma^0 = 323.15$ K; $a_1 = 1.6027$; $a_2 = 2.8235$; $b_1 = 982.27$, and $b_2 = 6861.39$.

Secondly, eqn. (5) can be utilized to take into account the effect of the other substances present on the ethanol activity coefficient [11].

$$\ln \frac{\gamma_e^s}{\gamma_e^0} = \delta_s x_s \qquad (5)$$

where γ_e^s is the ethanol activity coefficient in the presence of substance s, and x_e is the molar fraction of s in the liquid. Coefficient δ_s is constant for each substance; furthermore, it has been demonstrated that an additivity rule is fulfilled in the mixing of different compounds [12, 13]. Thus, a global coefficient γ_e is obtained from the following equation

$$\ln \frac{\gamma_e}{\gamma_e^0} = \sum_{s=1}^{n} \delta_s x_s \qquad (6)$$

Once the effect of substances present δ_s and their concentrations (x_s) are known, it is possible to calculate the global activity coefficient of ethanol. This means that it is necessary to monitor every x_s throughout the fermentation or, if no molar fraction changes greatly, to choose an average value.

The composition of the evolved gas can be calculated at any moment during the process using the equations cited above; however, it is necessary to know the ethanol evaporation rate to evaluate yield losses through evaporation. This rate depends not only on ethanol concentration in the gas phase, but also on the gas detachment velocity.

The gas detachment velocity can be considered equal to the carbon dioxide formation rate, as all the CO_2 formed is detached from the medium, and all other gas components are negligible compared with CO_2. Therefore, the ethanol evaporation rate is given by

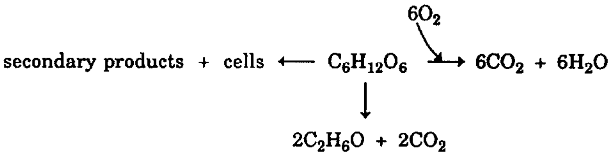
$$\frac{dE_{ev}}{dt} = y_e \frac{MW_e}{MW_c} \frac{dC}{dt} \qquad (7)$$

where MW_i is the molecular weight of the compound i; dE_{ev}/dt, the ethanol evaporation rate (in grammes per litre per hour); and dC/dt the carbon dioxide formation rate (in grammes per litre per hour).

Since the rate of ethanol evaporation can be calculated from eqn. (7), integrating this equation gives the yield losses owing to evaporation.

3. Combination of evaporation model with kinetic equations

It is necessary to combine the evaporation equation with the product formation kinetic equations so as to predict theoretically the kinetics of the industrial process. To obtain a more accurate model, yield losses owing to factors other than evaporation (*i.e.* respiration and other metabolite formation) have been considered. The kinetic model used is based on the following scheme of the fermentative process [2]



$$\text{secondary products} + \text{cells} \longleftarrow C_6H_{12}O_6 \xrightarrow{6O_2} 6CO_2 + 6H_2O$$

$$C_6H_{12}O_6 \longrightarrow 2C_2H_6O + 2CO_2$$

Consequently the following equations have been used [2]:

$$\frac{\mathrm{d}C}{\mathrm{d}t} = -2(f+3r)\frac{MW_c}{MW_s}\frac{\mathrm{d}S}{\mathrm{d}t} \qquad (8)$$

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -2f\frac{MW_e}{MW_s}\frac{\mathrm{d}S}{\mathrm{d}t}$$

where S is the substrate concentration (grammes per litre) and E is the ethanol concentration in the fermentation medium (grammes per litre). The constants f and r are the molar coefficients of fermentative and respiratory yields, respectively, and are temperature dependent according to the following Arrhenius equations

$$f = A_f \exp\left(-\frac{E_{f1}}{RT}\frac{T_f^0 - T}{T_f^0}\right) - B_f \exp\left(-\frac{E_{f2}}{RT}\frac{T_f^0 - T}{T_f^0}\right) \qquad (9)$$

$$r = A_r \exp\left(-\frac{E_{r1}}{RT}\frac{T - T_r^0}{T_r^0}\right) - B_r \exp\left(-\frac{E_{r2}}{RT}\frac{T - T_r^0}{T_r^0}\right)$$

where $A_f = 1.0769$; $B_f = 0.1287$; $E_{f1} = 2.4$ Kcal mol^{-1}; $E_{f2} = 20.0$ Kcal mol^{-1}; $T_f^0 = 295.9$ K; $A_r = 0.0490$; $B_r = 0.0182$; $E_{r1} = 6.7$ Kcal mol^{-1}; $E_{r2} = 18.0$ Kcal mol^{-1}, and $T_r^0 = 296.7$ K [2].

To obtain the combined equation it is necessary to introduce a transformation. Since in eqn. (7) the ethanol molar fraction in the medium is considered indirectly and in eqn. (8) a volumetric concentration is used, x_e can be substituted by a linear function of E [3]: $x_e = \alpha E$; where $\alpha = 4.021 \times 10^{-4}$ l g^{-1}. This makes the combined equation homogeneous and is a fair approximation in the concentration range reached during the process. Introducing the initial expressions produces the following general combined equation

$$\frac{\mathrm{d}E_{ev}}{\mathrm{d}t} = -2(f+3r)\,\alpha E\,\frac{p_e^0 \gamma_e}{p}\frac{MW_e}{MW_s}\frac{\mathrm{d}S}{\mathrm{d}t} \qquad (10)$$

To express E as a function of S it is necessary to integrate eqn. (8) for ethanol formation, assuming the coefficient f is a constant throughout the process. This is a fair approximation in industrial processes at fixed temperature, where the following integrated expression can be used

$$E = E_0 + 2f\frac{MW_e}{MW_s}(S_0 - S) \qquad (11)$$

S_0 and E_0 are the initial concentrations of substrate and ethanol respectively. Introducing eqn. (11) the general combined equation can be integrated if r and γ_θ are also considered constant throughout the process. Thus, the following combined equation is obtained

$$\mathrm{d}E_{ev} = (k_1 S - k_2)\,\mathrm{d}S$$

$$k_1 = 2f k_3 \frac{MW_e}{\mathrm{MW}_s} \qquad (12)$$

$$k_2 = k_3\left(E_0 + 2fS_0\frac{MW_e}{\mathrm{MW}_s}\right)$$

$$k_3 = 2(f+3r)\frac{p_e^0 \gamma_e \alpha}{p}\frac{MW_e}{MW_s}$$

Finally, integrating eqn. (12), results in the definitive evaporation expression

$$E_{ev} = K_1 S^2 + K_2 S + K_3$$

$$K_1 = \frac{k_1}{2} \qquad (13)$$

$$K_2 = -k_2$$

$$K_3 = k_2 S_0 - \frac{k_1}{2} S_0^2$$

The theoretical values of K_1, K_2, and K_3 can be calculated from the equations proposed above by introducing the corresponding operating conditions of each process. Using this evaporation equation it is possible to calculate the amount of ethanol evaporated (E_{ev}) from the start of the process until any moment, where the substrate concentration is S. The main objection arises in eqn. (6), since δ_s data are not available for every substance present in the medium.

TABLE 1. Values of ethanol activity coefficient increase constant (δ_s), for the ethanol–water system in the presence of different substances [11, 14]

Compound	δ_s
Potassium chloride	17.4
Sodium chloride	14.5
Ammonium chloride	11.0
Yeast extract	16.3[a]
Sodium nitrate	6.9
Potassium sulfate	2.3
Ammonium sulfate	8.1

[a] Calculated for concentration in grammes per millilitre.

4. Influence of substances present in the medium

Values of δ_s in eqn. (6) have been reported for several different substances under normal alcoholic fermentation conditions ($x_e < 0.05$, $x_s < 0.02$ and $T < 40$ °C) [11, 14]. Some of these values are shown in Table 1.

From the data available, it appears that the overall value of δ_s for salts is approximately 10. Therefore, for a common total salt concentration of 4 g l^{-1}, the value of the term $\Sigma\delta_s x_s$ would be 9×10^{-3}; and for a concentration of yeast of 10 g l^{-1} the corresponding value is 160×10^{-3}.

It is possible to ignore the effects of such salt concentrations. However, the possible effect of some of the other solutes present, such as sugars, tartaric acid, ethers or alcohols, must be considered. For this reason, it was necessary to carry out a series of laboratory experiments aimed at estimating the influence of such solutes on the ethanol activity coefficient.

4.1. Experimental details

The ethanol evaporation rate from aqueous solutions was studied using the apparatus shown in Fig. 1, in the presence of different compounds, and under the normal conditions of industrial alcohol fermentation (26 °C, $x_e < 0.05$ and CO_2 flow of 0.01 vvm).

To obtain global results for the induced effect, mixtures of heavy ethers (78 g l^{-1}), mixtures of light ethers with alcohols (932 g l^{-1}) and mixtures of sucrose (50 g l^{-1}) with tartaric acid (10 g l^{-1}) were studied. The compositions of the mixtures used are shown in Table 2.

In each case, the theoretical ethanol evaporation rate was calculated for a water–ethanol binary system under the experimental conditions, using eqns. (1)–(4) and (7). Experimental evaporation rates in the presence of the different mixtures were calculated from the chromatographic data of ethanol concentration in the exit stream of the absorption equipment. Utilizing eqn. (6), the value of the term $\Sigma\delta_s x_s$ was estimated from the ratio of theoretical and experimental data, corresponding to τ_e^s/τ_e^0. The results obtained are given in Table 3.

These data lead to an overall value for the corresponding term of 0.4, which shows the global effect of the substances studied. Consequently, it can be estimated that the order of the general activity ratio, under common industrial conditions, is 1.5.

5. Industrial scale model verification

To verify the theoretical model, several batch fermentations were carried out on an industrial scale (25 000 l) and at a controlled temperature of 26.5

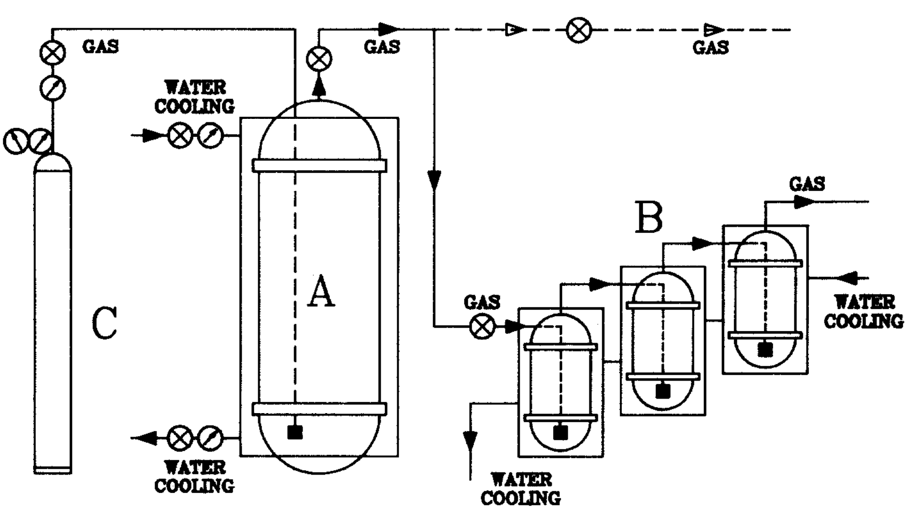


Fig. 1. Schematic of equipment utilized in laboratory experiments. (A) Batch fermenter; (B) absorption system, and (C) gas supply (CO_2).

TABLE 2. Composition of mixtures utilized for ethanol evaporation experiments (weight per cent)

Heavy ethers	%	Ethers and alcohols	%
Ethyl caproate	2.2	Acetaldehyde	38.0
Ethyl lactate	33.6	Methyl acetate	3.9
Ethyl caprilate	20.0	Ethyl acetate	10.1
Ethyl caprate	22.8	Methanol	5.6
Ethyl laurate	21.4	2-Butanol	1.3
		Propanol	6.4
		Iso-butanol	7.7
		Butanol	3.8
		Iso-amilic alcohol	23.2

TABLE 3. Values of $\delta_s x_s$ for each of the groups of compounds studied

Group	$\delta_s x_s$
Heavy ethers mixture	89×10^{-3}
Light ethers plus alcohols	74×10^{-3}
Sucrose plus tartaric acid	83×10^{-3}

°C. The equipment used is shown schematically in Fig. 2. The microorganism *Saccharomyces cerevisiae* var. cerevisiae was inoculated into a natural grape must (Palomino Fino variety). The operating conditions imposed were: initial substrate (sucrose), 172 g l^{-1}; initial viable biomass (dry weight), 30 mg l^{-1}; initial ethanol (present in the inoculum), 15 g l^{-1}.

The substrate concentration in the fermenter was measured periodically during the process by the dinitro-salicylic acid (DNS) method after hydrolysis [15], and the ethanol concentration was measured by gas chromatography [16]. Likewise, the ethanol concentration in the liquid leaving the gas absorption column was measured to determine the quantity of ethanol evaporated. The absorption column was operated in such a way that total ethanol retention was ensured. The results obtained are shown in Table 4.

Eqn. (13) was used to calculate theoretical evaporation for the experimental conditions. The values of constants utilized were obtained from the group of equations proposed (*i.e.* $K_1=2.4\times10^{-5}$, $K_2=-9.7\times10^{-3}$ and $K_3=1.0$). In eqn. (4), $x_e=1.8\times10^{-2}$ was used. This corresponds to the average ethanol molar fraction observed.

In Fig. 3, the experimental data obtained are shown *vs.* theoretical values. As can be observed, a good fit is obtained ($r^2=0.940$), demonstrating that the different factors of the evaporation phenomena have been successfully introduced into the model.

In addition, a least squares method has been used to obtain the values of the constants in eqn. (13) using the experimental data of substrate concentration and ethanol evaporated. The results obtained are as follows: $K_1=0.29\times10^{-5}$; $K_2=-5.99\times10^{-3}$, and $K_3=0.93$ ($r^2=0.981$). Good agreement between theoretical and experimental K values can be seen, K_1, which is of a much lower order of magnitude, only influences the initial stages of the

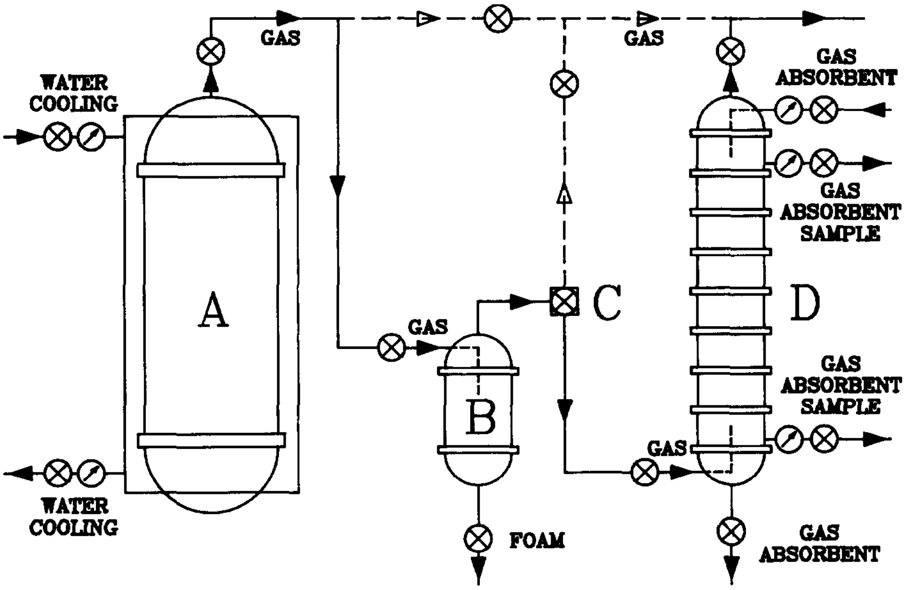


Fig. 2. Schematic of equipment utilized in industrial scale fermentation. (A) Batch fermenter; (B) foam knockout; (C) safety relief valve, and (D) absorption system.

TABLE 4. Experimental results of a batch alcoholic fermentation (industrial scale)

t (h)	S (g l^{-1})	E (g l^{-1})	E_{ev} (mg l^{-1})
0	172.1	15.0	0
3	171.6	14.8	0
4	171.6	17.2	0
16	158.6	22.2	107
18	148.5	22.3	124
20	139.9	26.1	142
22	138.6	33.3	160
23	123.1	39.5	179
24	131.8	36.4	197
25	110.3	42.0	218
26	102.9	43.0	238
28	114.5	42.6	279
30	108.4	47.2	333
39	81.2	66.8	519
41	63.5	69.8	560
43	61.0	72.9	601
44	66.9	68.9	622
46	56.8	71.6	648
47	47.5	76.6	661
49	40.6	77.7	686
52	39.7	78.3	725
54	34.8	84.7	744
57	30.0	86.5	769
59	26.9	88.2	785
63	21.7	88.5	802
65	21.7	88.5	811
67	18.2	88.7	819

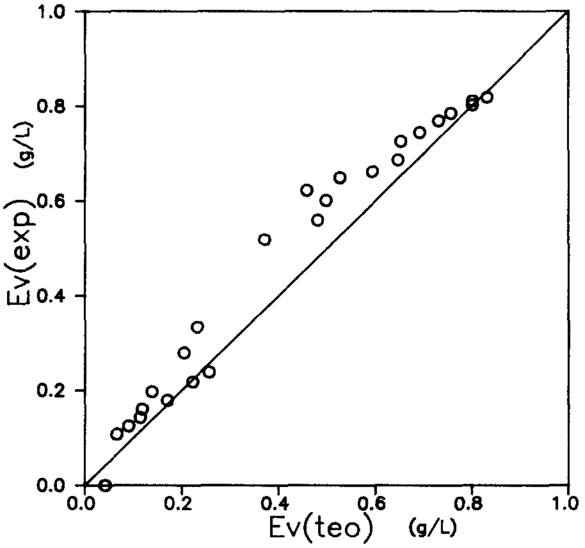


Fig. 3. Ethanol evaporation during the fermentation process. Experimental data *vs.* theoretical data (eqn. 3).

process. Deviations might be a result of simplifications and the averaging carried out during theoretical value estimation.

6. Influence of operating temperature

Equations describing the dependence of evaporation losses on temperature have been gathered from the literature. One of these has a theoretical basis [3]

$$\ln\left(\frac{E_{ev}}{S_0^2}\right)=A+\frac{B}{T} \tag{14}$$

In this case, the theoretical values of the proposed constants are $A=8.4090$ and $B=-5837$ (for E_{ev} and S_0, in grammes per litre, and T, in kelvins).

Another published relationship [4] has no theoretical justification, being entirely empirical

$$\ln\left(\frac{E_{ev}}{S_0^2}\right)=A+BT \tag{15}$$

In this expression, the values of the proposed constants depend on the initial substrate concentration.

Neither eqn. (14) nor (15) takes into account the influence of other yield loss factors on the evaporation losses; therefore, theoretical predictions of total yield losses could be wrong under some temperature conditions. To obtain a more general expression for the influence of temperature on the evaporative losses, eqn. (13) can be used, calculating the total evaporation losses at different temperatures. In this case $S=0$, since the substrate is assumed to have run out at the end of the process. The resulting expression is as follows

$$E_{ev}=k_3\left(E_0+2fS_0\frac{MW_e}{MW_s}\right)S_0-k_3\left(f\frac{MW_e}{MW_s}\right)S_0^2 \tag{16}$$

Replacing the k_3 value from eqn. (12), grouping terms and estimating the initial ethanol concentration to be negligible from the point of view of evaporation ($E_0=0$), results in the following equation

$$E_{ev}=p_e^0\gamma_e(f^2+3rf)\frac{2\alpha}{p}\frac{MW_e}{MW_s}S_0^2 \tag{17}$$

Rearrangement of eqn. (17) leads to

$$\ln\left(\frac{E_{ev}}{S_0^2}\right)=A+\phi_T$$

$$A=\ln\left[\frac{2\alpha}{p}\left(\frac{MW_e}{MW_s}\right)^2\right] \tag{18}$$

$$\phi_T=\ln[p_e^0\gamma_e(f^2+3rf)]$$

where parameters independent of temperature have been grouped into the constant A, the theoretical value of which is -16.488 (for E_{ev} and S_0, in grammes per litre, p, in millimetres of mercury, and T, in kelvins). The temperature dependent parameters f, r, p_e^0 and τ_e have been grouped into function ϕ_T, and must be calculated according to the equations given above. In eqn. (4), a value of $x_e = 2.2 \times 10^{-2}$ can normally be introduced, which corresponds to the average ethanol molar fraction expected from a typical initial substrate concentration ($S_0 = 216$ g l^{-1}).

6.1. Verification of the influence of temperature

To check the proposed eqn. (18), data from the literature corresponding to different batch fermentation processes and under different operating conditions, have been utilized. A summary of this data is shown in Table 5.

In order to establish comparisons among the different equations given above, the experimental and theoretical data for each equation have been plotted together in Fig. 4. For eqn. (15), to get a continuous curve, the values of the proposed constants have been calculated for $S_0 = 210$ g l^{-1}, which is the average value of the plotted data, this results in values: $A = -1.576 \times 10^{-4}$ and $B = 5.662 \times 10^{-7}$ for the same units as in eqn. (14).

It can be seen, from Fig. 4, that eqns. (14) and (15) predict a continuous increase of ethanol evaporation loss with increasing operating temperature. This effect is clearly not accurate since, at temperatures greater than 30 °C, other yield loss factors become significant, which makes both the ethanol concentration in the medium and the amount of CO_2 evolved much lower than expected by stoichiometry. It follows that total losses are lower as well. The model proposed here (eqn. (18)) does however predict losses properly under these conditions.

TABLE 5. Data on total evaporated ethanol for different batch alcoholic fermentation processes, compiled from the literature

T (K)	E_{ev} (g l^{-1})	S_0 (g l^{-1})	Ref.
5	0.15	183	17
10	0.10	220	18
11.3	0.18	160	19
15	0.80	214	2
20	1.10	214	2
20	0.55	182	17
21	0.42	220	18
21	0.55	276	18
21	0.68	276	18
22	0.47	216	20
25	1.40	214	2
26.5	0.86	172	2
26.5	0.58	220	18
27	0.86	265	21
28.5	0.52	204	22
29.5	0.07	177	23
30	1.80	214	2
30	0.56	115	21
32	0.80	220	18
34	1.30	276	18
35	1.30	214	2
35	1.03	182	17

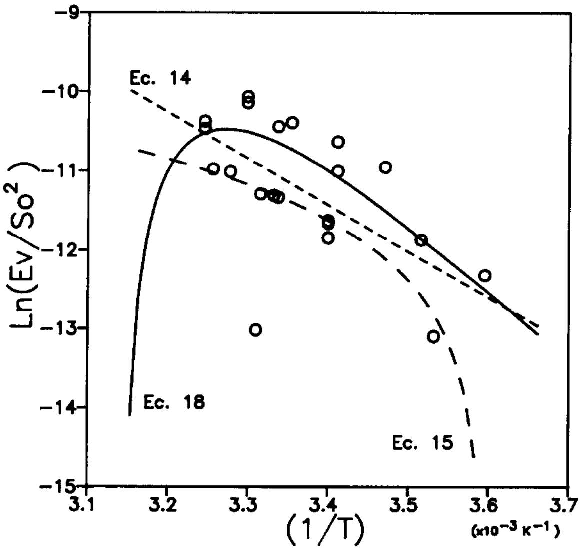


Fig. 4. Experimental data and different theoretical lines for total evaporated ethanol, over a range of operating temperatures.

It is interesting to note that, despite the relatively poor agreement between the individual data and the different equations ($r^2_{14} = 0.388$, $r^2_{15} = 0.292$, and $r^2_{18} = 0.346$), the theoretical expressions, *i.e.* eqns. (14) and (18), give generally better fits than the empirical relationship (eqn. (15)). In addition, the present model (eqn. (18)) offers a more likely prediction at high temperatures.

Predictions using eqn. (18) could suffer some discrepancies when modifying the τ_e/τ_e^0 value used, since not all fermentation substrates have the same composition characteristics. This could be one of the reasons why some of the experimental data show a different tendency to the theoretical curve. The constants used in eqn. (15) are similarly specific to a particular value of S_0; therefore, a different composition of fermentation substrate could also be the cause for deviations of the experimental data from this particular model.

It appears that, in general, eqn. (18) is superior to the others, both in its theoretical basis and in its fitting of extreme conditions. It therefore provides a better way to estimate likely evaporation yield losses.

7. Conclusions

The results obtained confirm the existence of different yield loss factors during industrial batch processes for alcohol production by fermentation; evaporation being one of them.

It has been demonstrated that these factors are not independent, but related to one another. For example, substances in the medium are liable to cause an increase in evaporation losses of about 50% compared with the ethanol–water binary system under the same conditions.

From the theoretical model proposed, a kinetic equation for yield losses by evaporation has been devised, this agrees closely with experimental data obtained on an industrial scale. The influence of operating temperature on the total evaporation yield losses during the process, is also predicted theoretically by the model, this presents an accurate fit to experimental data obtained under different conditions.

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Appendix A: Nomenclature

a, b, A, B	constants
C	amount of detached CO_2 (g l^{-1})
E	ethanol concentration in the medium (g l^{-1})
E_i	activation energy for process i (kcal mol^{-1})
E_{ev}	amount of evaporated ethanol (g l^{-1})
f	molar coefficient of fermentative conversion
MW	molecular weight
p	pressure of the gas phase (mmHg)
r	molar coefficient of respirative conversion
r^2	determination coefficient (regression analysis)
R	universal gas constant (kcal mol^{-1} k)
S	substrate concentration in the media (g l^{-1})
t	operating time (h)
T	operating temperature (K)
x	molar fraction in the liquid phase
y	molar fraction in the gas phase
α, k, K	parameters considered to be constant
δ	increase of ethanol activity coefficient
τ	activity coefficient in the liquid phase

Subscripts

e	ethanol
i	compound i
s	substrate
t	total
0	initial

Superscripts

s	in the presence of salt
0	referred to pure compounds