

Derivation and Application of a Simultaneous Volatile Formation and Stripping Kinetics Equation for Wort Boiling

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ABSTRACT

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The paper showed the derivation of an equation to represent simultaneous dimethyl sulfide (DMS) formation and stripping during wort boiling. It also demonstrated a framework of linearization techniques for the resulting equation, which should facilitate its implementation. DMS formation and stripping were modelled by first-order rate equations with the rate constants k_1 and k_2 representing the rate constants for rate of DMS formation and DMS removal via stripping, respectively. The simultaneous processes of DMS formation and stripping were represented using an instantaneous differential mass balance. The resulting solution was seen to be similar to an equation stated previously by Mitani et al. Linearization of the derived simultaneous DMS formation and stripping model was done using a MacLaurin series coming from Taylor's series expansion.

Keywords: Dimethyl sulfide, *S*-Methylmethionine, Wort boiling, Volatile formation, Volatile stripping, Nonlinear MacLaurin series

Dimethyl sulfide (DMS) is a standout among the most critical off-flavors in the mashing process (1–3,6,12,16,21,26,30); the stripping of that unstable volatile is an exceptionally complex procedure, and it is made of two synchronous reactions, which are the change of *S*-methylmethionine (SMM) into DMS and its stripping (5,17). That difficult circumstance created numerous sorts of methodologies as far as boiling vessels and equations so as to handle disposal of DMS (8–11,19,20,23,24,27,28). For that reason, the principal model known for DMS stripping is the one of Mitani et al. (23,24), which is of a nonlinear form. Such nonlinear models are frequently linearized to ease implementation.

In this work, the detailed derivation of a simultaneous DMS formation and stripping model is described, and the final nonlinear model is compared with the model stated by Mitani et al. (23) and found to be identical in form. To facilitate implementation, linearization of the nonlinear model was conducted using a MacLaurin–Taylor series expansion.

EXPERIMENTAL

Derivation of a DMS Stripping Model

In these methods differential equations that gave the conversion of SMM to DMS and DMS stripping with time ($d[SMM]/dt$ and $d[DMS]/dt$) were integrated to give a rate equation that followed the concentration of SMM or DMS elimination (stripping) as a function of time.

MacLaurin Series Approach for SMM and DMS Nonlinear Models

The MacLaurin series (which is a particular Taylor series when $x_0 = 0$) is utilized to approximate infinitely differentiable nonlinear equations. The MacLaurin polynomial function is built up

according to the derivatives of the SMM and DMS functions at a 0. The main idea behind the MacLaurin series is as follows: Derivatives, practically speaking, correlate to the contour of a curve, so the higher derivatives that two models have similarly at one point (0), the more comparable they appear at other nearby points (7,22). MacLaurin series are essential because they permit the figuring out of models that could not be computed directly or are difficult to handle. Although the MacLaurin polynomial for the exponential model seems confusing and irritating, it can be reduced to addition, subtraction, multiplication, and division. One can acquire an estimate of the original function by truncating the infinite MacLaurin series into a limited-degree MacLaurin polynomial, which can be assessed.

Determination of Constants: $[SMM]_{t=0}$, $[DMS]_{t=0}$, k_1 , and k_2

The methodology consists of, on the first hand (for each case, SMM and DMS), determining the best polynomial equation that correlates the experimental data. For each case, the obtained polynomial equation allows the determination of $[SMM]_{t=0}$ and $[DMS]_{t=0}$ via its constant. The constant value of the derivate polynomial equation for each case permits the calculation of k_1 and k_2 .

RESULTS AND DISCUSSION

Derivative Approach of Establishing DMS Stripping Model

Most chemical reactions take place in several stages; that is to say they evolve by successive elementary chemical reactions in which each step has its own rate with respect to time. DMS elimination from wort can also be considered the result of two consecutive irreversible reactions (namely, SMM conversion into DMS and thereafter DMS volatilization). The rate of each reaction can be considered to be concentration dependent, and more specifically as a first-order reaction, in which the rate of progress of each reaction with respect to time is proportional to the concentration of the reactant, where the constant of proportionality (k) is termed the reaction rate coefficient (31). These consecutive reactions are presented as follows: $SMM \xrightarrow{k_1} DMS \xrightarrow{k_2} DMS^{evap}$, where k_1 is the reaction rate coefficient of SMM conversion to DMS and k_2 is the volatilization rate coefficient of DMS.

Considering the depletion of SMM as a first-order reaction, where the concentration of SMM at any time t , denoted as $[SMM]_t$, is proportional to the concentration of SMM,

$$-\frac{d[SMM]_t}{dt} = k_1 [SMM]_t = k_1 [SMM]_t \quad (1)$$

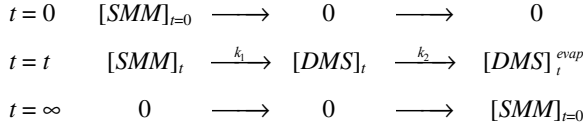
The negative sign is owing to depletion, and the first-order refers to the power index = 1.

Because the DMS produced, which is denoted $[DMS]_t^{prod}$, increases with time and is also proportional to the concentration of SMM, it is then expressed with a positive as follows:

$$\frac{d[DMS]_t^{prod}}{dt} = k_1 [SMM]_t = k_1 [SMM]_t \quad (2)$$

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The reaction conditions are as follows:



where $[SMM]_{t=0}$ is the initial SMM concentration, before the boiling stage.

In a similar way to $[DMS]_t^{prod}$, the concentration of volatized DMS, denoted as $[DMS]_t^{evap}$, increases with time and is proportional to the concentration of DMS. It is then expressed with a positive sign as follows:

$$\frac{d[DMS]_t^{evap}}{dt} = k_2 [DMS]_t = k_2 [DMS]_t \quad (3)$$

The rate of $[DMS]_t$ remaining in the wort owing to the consecutive reactions is expressed as the difference between the rate of SMM conversion to DMS and the rate of DMS volatilized denoted $[DMS]_t^{evap}$:

$$\frac{d[DMS]_t}{dt} = \frac{d[DMS]_t^{prod}}{dt} - \frac{d[DMS]_t^{evap}}{dt} = k_1 [SMM] - k_2 [DMS] \quad (4)$$

With respect to the mass balance, the initial concentration of SMM, denoted $[SMM]_{t=0}$, can be expressed at any time as follows:

$$[SMM]_t + [DMS]_t + [DMS]_t^{evap} = [SMM]_{t=0} \quad (5)$$

Rearranging equation 1 gives

$$\frac{d[SMM]_t}{[SMM]_t} = -k_1 dt \quad (6)$$

By integrating both sides of equation 5 we get

$$\int_{[SMM]_{t=0}}^{[SMM]_t} \frac{d[SMM]_t}{[SMM]_t} = -\int_0^t k_1 dt \Rightarrow \int_{[SMM]_{t=0}}^{[SMM]_t} \frac{1}{[SMM]_t} d[SMM]_t = -\int_0^t k_1 dt \quad (7)$$

where $[SMM]_{t=0}$ is the initial SMM concentration, before the boiling stage.

After completing integration and from the law of logarithms we obtain

$$\ln[SMM]_t - \ln[SMM]_{t=0} = -k_1 t \Rightarrow \ln\left(\frac{[SMM]_t}{[SMM]_{t=0}}\right) = -k_1 t \quad (8)$$

A transformation of the equation 8 gives

$$\ln\left(\frac{[SMM]_t}{[SMM]_{t=0}}\right) = -k_1 t \Leftrightarrow \exp\left(\ln\left(\frac{[SMM]_t}{[SMM]_{t=0}}\right)\right) = \exp(-k_1 t) \quad (9)$$

When simplifying equation 9, the rate law becomes

$$\frac{[SMM]_t}{[SMM]_{t=0}} = \exp(-k_1 t) \Rightarrow [SMM]_t = [SMM]_{t=0} \exp(-k_1 t) \quad (10)$$

To determine $[DMS]_t$ remaining in the system during the two consecutive reactions, equation 4 is used. After rearranging that equation, the relation obtained is as follows:

$$\begin{aligned} \frac{d[DMS]_t}{dt} &= k_1 [SMM]_t - k_2 [DMS]_t \\ &\Rightarrow \frac{d[DMS]_t}{dt} + k_2 [DMS]_t = k_1 [SMM]_t \end{aligned} \quad (11)$$

Substituting the expression for $[SMM]_t$, equation 10, into equation 11 gives

$$\frac{d[DMS]_t}{dt} + k_2 [DMS]_t = k_1 [SMM]_{t=0} \exp(-k_1 t) \quad (12)$$

Let us consider the following relation in order to understand and use equation 12:

$$\frac{d}{dt}([DMS]_t \exp(k_2 t)) \quad (13)$$

Recall that mathematical calculus states

$$\begin{aligned} \frac{d}{dx}[f(x)\exp(g(x))] &= \exp(g(x)) \frac{d}{dx}(f(x)) \\ &+ f(x) \frac{d}{dx}(\exp(g(x))) \end{aligned} \quad (14)$$

So equation 13 can be rewritten as

$$\begin{aligned} \frac{d}{dt}([DMS]_t \exp(k_2 t)) &= \exp(k_2 t) \frac{d[DMS]_t}{dt} \\ &+ [DMS]_t \frac{d}{dt}(\exp(k_2 t)) \end{aligned} \quad (15)$$

Then, we obtain from equation 15 the following relation:

$$\begin{aligned} \exp(k_2 t) \frac{d[DMS]_t}{dt} + [DMS]_t \frac{d}{dt}(\exp(k_2 t)) \\ = \exp(k_2 t) \frac{d[DMS]_t}{dt} + k_2 [DMS]_t \exp(k_2 t) \end{aligned} \quad (16)$$

Finally, it can be written as

$$\frac{d}{dt}([DMS]_t \exp(k_2 t)) = \exp(k_2 t) \frac{d[DMS]_t}{dt} + k_2 [DMS]_t \exp(k_2 t) \quad (17)$$

By distributing $\exp(k_2 t)$ in equation 17, we get the following:

$$\frac{d}{dt}([DMS]_t \exp(k_2 t)) = \exp(k_2 t) \left(\frac{d[DMS]_t}{dt} + k_2 [DMS]_t \right) \quad (18)$$

Considering the right hand-side of equation 18 only, and substituting the result of equation 12 for the term within the large brackets gives

$$\exp(k_2 t) \left(\frac{d[DMS]_t}{dt} + k_2 [DMS]_t \right) = k_1 [SMM]_{t=0} \exp(-k_1 t) \exp(k_2 t) \quad (19)$$

By rearranging equation 19, we have

$$\exp(k_2 t) \left(\frac{d[DMS]_t}{dt} + k_2 [DMS]_t \right) = k_1 [SMM]_{t=0} \exp((k_2 - k_1)t) \quad (20)$$

Substituting equation 20 into equation 18 gives

$$\frac{d}{dt} ([DMS]_t \exp(k_2 t)) = k_1 [SMM]_{t=0} \exp((k_2 - k_1)t) \quad (21)$$

Rearranging equation 21 gives

$$d([DMS]_t \exp(k_2 t)) = k_1 [SMM]_{t=0} \exp((k_2 - k_1)t) dt \quad (22)$$

Integrating both sides, we obtain the following relation:

$$\int_0^{[DMS]_t \exp(k_2 t)} d([DMS]_t \exp(k_2 t)) = k_1 [SMM]_{t=0} \int_0^t \exp((k_2 - k_1)t) dt \quad (23)$$

(Note that the lower limit of the left-hand integral at $t = 0$ reduces to 0.)

Continuing on, we know that

$$\int_0^{[DMS]_t \exp(k_2 t)} d([DMS]_t \exp(k_2 t)) = \left[[DMS]_t \exp(k_2 t) \right]_0^{[DMS]_t \exp(k_2 t)} = [DMS]_t \exp(k_2 t) \quad (24)$$

We know also that

$$\int_0^t \exp((k_2 - k_1)t) dt = \left[\frac{1}{(k_2 - k_1)} \exp((k_2 - k_1)t) \right]_0^t = \left(\frac{1}{(k_2 - k_1)} [\exp((k_2 - k_1)t) - 1] \right) \quad (25)$$

After combining equations 24 and 25 with equation 23, we can then write

$$[DMS]_t \exp(k_2 t) = k_1 [SMM]_{t=0} \left(\frac{1}{(k_2 - k_1)} [\exp((k_2 - k_1)t) - 1] \right) \quad (26)$$

Then,

$$[DMS]_t = k_1 [SMM]_{t=0} \left(\frac{1}{(k_2 - k_1)} [\exp((k_2 - k_1)t) - 1] \right) \exp(-k_2 t) \quad (27)$$

After using exponential laws and expanding equation 27, we obtain the following:

$$[DMS]_t = \left[\frac{k_1 [SMM]_{t=0}}{(k_2 - k_1)} [\exp((k_2 - k_1 - k_2)t) - \exp(-k_2 t)] \right] \quad (28)$$

After simplifying equation 28, the relation obtained is

$$[DMS]_t = \left[\frac{k_1 [SMM]_{t=0}}{(k_2 - k_1)} (\exp(-k_1 t) - \exp(-k_2 t)) \right] \quad (29)$$

In a real situation, at the end of mashing, the wort contains a certain amount of DMS coming from the conversion of SMM

during the mashing process ($[DMS]_t^{mash}$), and it is also reduced by volatilization during the boiling stage. That additional DMS in the wort follows also the first-order kinetic, and therefore it is expressed as follows:

$$[DMS]_t^{mash} = [DMS]_{t=0} \exp(-k_2 t) \quad (30)$$

where $[DMS]_{t=0}$ is the initial DMS concentration, before the boiling stage.

The total concentration of DMS residual in the wort (denoted $[DMS]_t^{total}$) at the end of the boiling phase is, therefore, in respect of mass balance, equal to the residual DMS owing to the two consecutive irreversible reactions ($[DMS]_t$) during wort boiling, to which is added the residual amount of DMS coming from the conversion of SMM during mashing ($[DMS]_t^{mash}$). It is expressed as follows:

$$[DMS]_t^{total} = [DMS]_t^{mash} + [DMS]_t \quad (31)$$

Knowing the expressions of $[DMS]_t$ from equation 29 and the one of $[DMS]_t^{mash}$ from equation 30, the total amount of DMS ($[DMS]_t^{total}$) could be written from equation 31 as follows:

$$[DMS]_t^{total} = [DMS]_{t=0} \exp(-k_2 t) + \left[\frac{k_1 [SMM]_{t=0}}{(k_2 - k_1)} (\exp(-k_1 t) - \exp(-k_2 t)) \right] \quad (32)$$

where $[DMS]_0$ and $[SMM]_0$ are the initial DMS and SMM concentrations, respectively, k_1 is the reaction rate coefficient of SMM conversion to DMS, and k_2 is the volatilization rate coefficient of DMS.

Equation 32 developed from reaction kinetics and for DMS stripping was identical in form to that of Mitani et al. (23).

MacLaurin Series Approximations for SMM and DMS Nonlinear Models

MacLaurin series approach. The linearization is done using the MacLaurin series, which is a particular expression of a Taylor series. That Taylor series is expressed as follows (4,7,14,29):

$$f(t) = \sum_{n=0}^{\infty} \frac{f^{(n)}(t_0)}{n!} (t - t_0)^n \quad (33)$$

The most typical form of useful sequence is the power series, which employs powers of the separate variables as basic functions. The first kind of polynomial series is the MacLaurin series (25):

$$f(t) = s(t) = a_0 + a_1 t + a_2 t^2 + \dots + a_{n-1} t^{n-1} + a_n t^n \quad (34)$$

whereby $f(t)$ (the function to be symbolized) and $s(t)$ hold for the series. We want then to identify the coefficients. As a way for the function and the series to be equivalent at all values of t in some interval as well as $t = 0$, they need to be identical at $t = 0$, which suggests that all of the terms in the series disappear apart from the following for the first expression:

$$f(0) = s(0) = a_0 \quad (35)$$

This decides a_0 . To be able to illustrate a function by a power series, we need that the function and all of its derivatives remain differentiable at $t = 0$. This kind of a function is stated to be logical at $t = 0$. After that, it is needed to have all derivatives of the

function as well as the series equate at $t = 0$. The n th derivation of the series at $t = 0$ is

$$\left(\frac{d^n s}{dt^n}\right)_{t=0} = n!a_n \quad (36)$$

where $n!$ (n factorial) is prescribed for $n \geq 1$ and for instance (18)

$$n! = n(n-1)(n-2)(n-3)(n-4)\cdots(4)(3)(2)(1) \quad (37)$$

where $0!$ is considered to be equal to 1 based to the agreement for an empty product (15). The standard formula for the MacLaurin series coefficients to characterize the function $f(t)$ is therefore

$$a_n = \frac{1}{n!} \left(\frac{d^n f}{dt^n}\right)_{t=0} = \frac{1}{n!} (f^{(n)})_{t=0} = \frac{1}{n!} f^{(n)}(0) \quad (38)$$

$(n = 1, 2, 3, 4, 5, 6, \dots)$

The MacLaurin series development for $f(t)$ around $t = 0$ therefore evolves into (7,22)

$$f(t) = f(0) + \frac{f^{(1)}(0)}{1!}t + \frac{f^{(2)}(0)}{2!}t^2 + \frac{f^{(3)}(0)}{3!}t^3 + \frac{f^{(4)}(0)}{4!}t^4 + \dots + \frac{f^{(n)}(0)}{n!}t^n \quad (39)$$

Then, that power series could be expressed in complete form, by using the sum symbol as follows:

$$f_\infty(t) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} (t^n) \quad (40)$$

Approximating $[SMM]_t$ and $[DMS]_t$ total nonlinear models using the MacLaurin series. Let us now consider equations 10 and 32, which are exponential functions. To be able to transform them as a power series (equation 38), it is therefore necessary to derive these nonlinear functions and expand them around $t = 0$.

Let us define these nonlinear functions (equations 10 and 32) as follows:

$$[SMM]_t = g(t) = [SMM]_{t=0} \exp(-k_1 t) \quad (41)$$

and

$$[DMS]_t^{\text{total}} = h(t) = [DMS]_{t=0} \exp(-k_2 t) + \left[\frac{k_1 [SMM]_{t=0}}{(k_2 - k_1)} (\exp(-k_1 t) - \exp(-k_2 t)) \right] \quad (42)$$

The values of $g(t)$ and $h(t)$ around $t = 0$ and expressed respectively by $g(0)$ and $h(0)$ are

$$g(0) = [SMM]_{t=0} \quad (43)$$

$$h(0) = [DMS]_{t=0} \quad (44)$$

Recall from mathematical calculus that

$$f^{(n)}(x) = \frac{d^n}{dx^n} (f(x)) = \frac{d}{dx} (f^{(n-1)}(x)) \quad (45)$$

and

$$\begin{aligned} \frac{d}{dx} (a \exp(f(x))) &= a \left(\frac{d}{dx} f(x) \right) \exp(f(x)) \\ &= a [f'(x)] \exp(f(x)) \end{aligned} \quad (46)$$

So by doing successive derivations of equations 41 and 42, we have the following series of derivations:

first derivation:

$$g^{(1)}(t) = -[SMM]_{t=0} k_1 \exp(-k_1 t) \quad (47)$$

$$\begin{aligned} h^{(1)}(t) &= [SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1 \exp(-k_1 t) - k_2 \exp(-k_2 t)) \\ &\quad - [DMS]_{t=0} k_2 \exp(-k_2 t) \end{aligned} \quad (48)$$

second derivation:

$$g^{(2)}(t) = k_1^2 [SMM]_{t=0} \exp(-k_1 t) \quad (49)$$

$$h^{(2)}(t) = - \left([SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^2 \exp(-k_1 t) - k_2^2 \exp(-k_2 t)) - [DMS]_{t=0} k_2^2 \exp(-k_2 t) \right) \quad (50)$$

third derivation:

$$g^{(3)}(t) = -k_1^3 [SMM]_{t=0} \exp(-k_1 t) \quad (51)$$

$$\begin{aligned} h^{(3)}(t) &= [SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^3 \exp(-k_1 t) - k_2^3 \exp(-k_2 t)) \\ &\quad - [DMS]_{t=0} k_2^3 \exp(-k_2 t) \end{aligned} \quad (52)$$

fourth derivation:

$$g^{(4)}(t) = k_1^4 [SMM]_{t=0} \exp(-k_1 t) \quad (53)$$

$$h^{(4)}(t) = - \left([SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^4 \exp(-k_1 t) - k_2^4 \exp(-k_2 t)) - [DMS]_{t=0} k_2^4 \exp(-k_2 t) \right) \quad (54)$$

⋮

n th derivation:

$$g^{(n)}(t) = (-1)^n [SMM]_{t=0} k_1^n \exp(-k_1 t) \quad (55)$$

$$h^{(n)}(t) = (-1)^n \left([SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^n \exp(-k_1 t) - k_2^n \exp(-k_2 t)) - [DMS]_{t=0} k_2^n \exp(-k_2 t) \right) \quad (56)$$

where $n \geq 1$.

The calculus of the derivative functions around $t = 0$ ($g^{(n)}(0)$ and $h^{(n)}(0)$), and with $n = 1, 2, 3, \dots$ are then expressed as in the following series of derivations:

first derivation:

$$g^{(1)}(0) = -[SMM]_{t=0} k_1 \quad (57)$$

$$h^{(1)}(0) = k_1 [SMM]_{t=0} - k_2 [DMS]_{t=0} \quad (58)$$

second derivation:

$$g^{(2)}(0) = k_1^2 [SMM]_{t=0} \quad (59)$$

$$h^{(2)}(0) = - \left([SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^2 - k_2^2) - [DMS]_{t=0} k_2^2 \right) \quad (60)$$

third derivation:

$$g^{(3)}(0) = -k_1^3 [SMM]_{t=0} \quad (61)$$

$$h^{(3)}(0) = \left([SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^3 - k_2^3) - [DMS]_{t=0} k_2^3 \right) \quad (62)$$

fourth derivation:

$$g^{(4)}(0) = k_1^4 [SMM]_{t=0} \quad (63)$$

$$h^{(4)}(0) = - \left([SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^4 - k_2^4) - [DMS]_{t=0} k_2^4 \right) \quad (64)$$

⋮

n th derivation:

$$g^{(n)}(0) = (-1)^n k_1^n [SMM]_{t=0} \quad (65)$$

$$h^{(n)}(0) = (-1)^n \left[[SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^n - k_2^n) - [DMS]_{t=0} k_2^n \right] \quad (66)$$

where $n \geq 1$.

The power series of $[SMM]_t$ and $[DMS]_t^{total}$ is then expressed as follows:

$$\begin{aligned} [SMM]_t &= [SMM]_{t=0} - \frac{([SMM]_{t=0} k_1)}{1!} t \\ &+ \left(\frac{[SMM]_{t=0} k_1^2}{2!} \right) t^2 - \left(\frac{[SMM]_{t=0} k_1^3}{3!} \right) t^3 \\ &+ \left(\frac{[SMM]_{t=0} k_1^4}{4!} \right) t^4 + \dots + \left(\frac{(-1)^n k_1^n [SMM]_{t=0}}{n!} \right) t^n \end{aligned} \quad (67)$$

$$\begin{aligned} [DMS]_t^{total} &= [DMS]_{t=0} + \frac{([SMM]_{t=0} k_1 - [DMS]_{t=0} k_2)}{1!} t \\ &- \frac{\left([SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^2 - k_2^2) - [DMS]_{t=0} k_2^2 \right)}{2!} t^2 \\ &+ \frac{\left([SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^3 - k_2^3) - [DMS]_{t=0} k_2^3 \right)}{3!} t^3 \\ &- \frac{\left([SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^4 - k_2^4) - [DMS]_{t=0} k_2^4 \right)}{4!} t^4 + \dots \\ &+ \frac{(-1)^n \left[[SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^n - k_2^n) - [DMS]_{t=0} k_2^n \right]}{n!} t^n \end{aligned} \quad (68)$$

Determination of SMM and DMS Equations Constants

In this section, the aim is to ease the determination of constant coefficients of $[SMM]_t$ and $[DMS]_t^{total}$ nonlinear functions by means of linearization using the MacLaurin series. That transformation of nonlinear functions into power series could be one of the solutions to coefficient determination because that series looks much easier to handle.

Use of nonlinear equation for determination of constants. The constants to be determined here are k_1 , k_2 , $[SMM]_{t=0}$, and $[DMS]_{t=0}$.

From the nonlinear equation of $[SMM]_t$, it is possible to determine k_1 and $[SMM]_{t=0}$ by using the logarithm:

$$\begin{aligned} [SMM]_t &= [SMM]_{t=0} \exp(-k_1 t) \Rightarrow \ln([SMM]_t) \\ &= \ln([SMM]_{t=0} \exp(-k_1 t)) \end{aligned} \quad (69)$$

Recall from logarithm laws that

$$\ln(ab) = \ln(a) + \ln(b) \quad (70)$$

$$\ln(\exp(a)) = a \quad (71)$$

From these laws, it is written

$$\begin{aligned} \ln([SMM]_t) &= \ln([SMM]_{t=0} \exp(-k_1 t)) \Rightarrow \ln([SMM]_t) \\ &= \ln([SMM]_{t=0}) + \ln(\exp(-k_1 t)) \end{aligned} \quad (72)$$

$$\begin{aligned} \ln([SMM]_t) &= \ln([SMM]_{t=0}) + \ln(\exp(-k_1 t)) \\ &\Rightarrow \ln([SMM]_t) = \ln([SMM]_{t=0}) - k_1 t \end{aligned} \quad (73)$$

From equation 73, it is observed that the introduction of the logarithm transformed it into a linear form in which $\ln[SMM]_{t=0}$ is obtained when $t = 0$ and $-k_1$ is the slope after obtaining the linear regression equation from the experimental data, when plotting $\ln([SMM]_t) = f(t)$. An illustration is presented in Figure 1.

For the $[DMS]_t^{total}$ equation, the determination of k_2 and $[DMS]_{t=0}$ are the main concern because k_1 and $[SMM]_{t=0}$ are already estimated. For this case, the structure of that nonlinear equation 42 is so complex that an easy way of determining the constants is diffi-

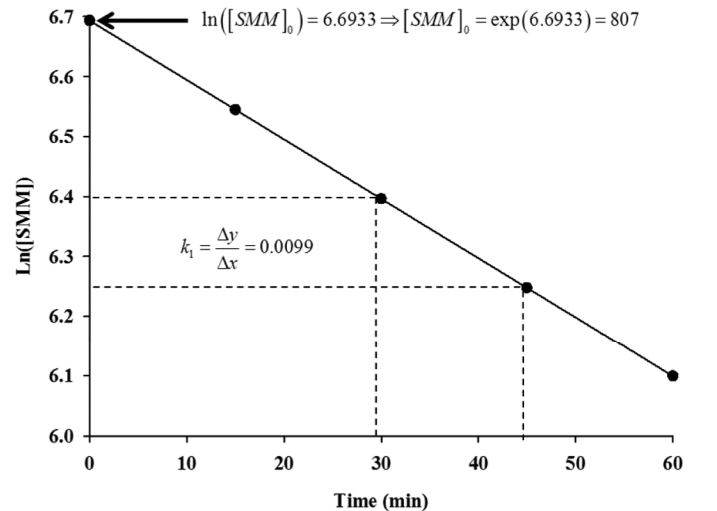


Fig. 1. Simplification of *S*-methylmethionine (SMM) nonlinear equation using logarithm.

cult to implement. For that purpose, we need to apply nonlinear regression fitting, but that is possible only with specific software such as Sigmaplot, Matlab, or BrainMaker, for which a program must be written for these software packages to solve the equation and give the desired results. This last software (BrainMaker version 2.3) was used by Mitani et al. in 1999 (23). This justifies thereby the necessity of finding another way of acquiring these data.

Use of power series for determination of constants. For $[SMM]_t$ equation constants determination, equation 67 is considered. When fitting that equation with the experimental data, we then deduce graphically that the value of $[SMM]_{t=0}$ is obtained at $t = 0$. By making a correspondence with the MacLaurin series of equation 34, we can therefore state that

$$[SMM]_{t=0} = a_0 \quad (74)$$

After obtaining the value of $[SMM]_{t=0}$, the remaining constant to determine for the $[SMM]_t$ equation is k_1 . One of the ways of determining it is graphically after deriving the $[SMM]_t$ equation and plotting the derivation. Deriving of equation 67 gives the following:

$$\begin{aligned} \frac{d}{dt}[SMM]_t = & -([SMM]_{t=0} k_1) + 2\left(\frac{[SMM]_{t=0} k_1^2}{2!}\right)t \\ & - 3\left(\frac{[SMM]_{t=0} k_1^3}{3!}\right)t^2 + 4\left(\frac{[SMM]_{t=0} k_1^4}{4!}\right)t^3 \\ & + \dots + n\left(\frac{(-1)^n k_1^n [SMM]_{t=0}}{n!}\right)t^{n-1} \end{aligned} \quad (75)$$

An analysis of equation 75 permits stating that, by plotting it, the value of $-([SMM]_{t=0} k_1)$ is obtained at $t = 0$. By comparing that equation 75 to the derivative equation of the MacLaurin series (equation 34), which is expressed as

$$\begin{aligned} \frac{d}{dt}(f(t)) = f^{(1)}(t) = & a_1 + 2a_2t + 3a_3t^2 + \dots \\ & + (n-1)a_{n-1}t^{n-2} + na_n t^{n-1} \end{aligned} \quad (76)$$

we can say that

$$\left[-([SMM]_{t=0} k_1)\right] = a_1 \quad (77)$$

Knowing that $[SMM]_{t=0} = a_0$, we can then finally have

$$\left[-([SMM]_{t=0} k_1)\right] = a_1 \Rightarrow -a_0 k_1 = a_1 \Rightarrow k_1 = -\frac{a_1}{a_0} \quad (78)$$

For $[DMS]_t^{total}$ equation constants, the same approach is used. For this case, the constants to determine are k_2 and $[DMS]_{t=0}$, knowing that k_1 and $[SMM]_{t=0}$ are already determined. The approach again is to fit the $[DMS]_t^{total}$ power series approximation (equation 68) with experimental data. By that method, the value of $[DMS]_{t=0}$ is obtained at $t = 0$. If the MacLaurin series is rewritten as follows

$$f(t) = b_0 + b_1t + b_2t^2 + \dots + b_{n-1}t^{n-1} + b_n t^n \quad (79)$$

we can then write by comparison of equations 68 and 79 that

$$[DMS]_{t=0} = b_0 \quad (80)$$

When deriving $[DMS]_t^{total}$ and the MacLaurin power series equations, we obtain

$$\begin{aligned} \frac{d}{dt}([DMS]_t^{total}) = & ([SMM]_{t=0} k_1 - [DMS]_{t=0} k_2) \\ & - \left([SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^2 - k_2^2) - [DMS]_{t=0} k_2^2\right)t + \dots \\ & + n \frac{(-1)^n \left[-([SMM]_{t=0} \frac{k_1}{k_1 - k_2} (k_1^n - k_2^n) - [DMS]_{t=0} k_2^n)\right]}{n!} t^{n-1} \end{aligned} \quad (81)$$

$$\frac{d}{dt}(f(t)) = f^{(1)}(t) = b_1 + 2b_2t + \dots + (n-1)b_{n-1}t^{n-2} + nb_n t^{n-1} \quad (82)$$

By comparing the two derivative equations 81 and 82, we deduce the following:

$$([SMM]_{t=0} k_1 - [DMS]_{t=0} k_2) = b_1 \quad (83)$$

That value of b_1 is obtained when the derivative equation 76 is around $t = 0$. The value of k_2 is then calculated from equation 77 as the following:

$$\begin{aligned} ([SMM]_{t=0} k_1 - [DMS]_{t=0} k_2) = b_1 \Rightarrow [DMS]_{t=0} k_2 \\ = ([SMM]_{t=0} k_1) - b_1 \end{aligned} \quad (84)$$

Then,

$$k_2 = \frac{([SMM]_{t=0} k_1) - b_1}{[DMS]_{t=0}} \quad (85)$$

Application of the MacLaurin Series on Evaluating Reaction Rate Coefficient of SMM Conversion to DMS (k_1), Initial SMM Concentration ($[SMM]_{t=0}$), Initial DMS Concentration ($[DMS]_{t=0}$), and Volatilization Rate Coefficient (k_2)

In this part, we provide a range of illustrative cases to exhibit the use of equations 66 and 67. In all of these cases concerning wort boiling, we have applied MacLaurin series approximation of the functions to resolve k_1 , k_2 , $[SMM]_{t=0}$, and $[DMS]_{t=0}$. All the polynomial regressions were done using CurveExpert Professional version 2.3 software (©2011–2016 Daniel G. Hyams) and verified with TableCurve 2D version 5.01 software (Systat Software, San Jose, CA, U.S.A.). The method in all the subsequent cases is identical.

First, the linearized equation is built into experimental data as a way to figure out $[SMM]_{t=0}$. Second, the linearized equation is derived and the formula obtained is plotted to be able to determine k_1 . Third, the linearized model of $[DMS]_t^{total}$ evolution is also fitted to its experimental data to determine $[DMS]_{t=0}$. Finally, that equation is derived, and the derivative equation is one more time plotted to calculate the value of k_2 , being aware of the values of k_1 , $[SMM]_{t=0}$, and $[DMS]_{t=0}$.

Example 1. Let us consider Mitani et al. (23) wort boiling experimental data obtained after using a pilot-scale kettle with a volume of 0.4 m³, heat exchange area of 0.3 m³, and heat supply rate of 160 MJ·m⁻³·wort·h⁻¹. That wort boiling process is realized for 90 min, and the data are compiled in Table I. Figures 2A and 3A show that the power series having the best regression with the experimental data is in both cases the third-order polynomial equation. These third-order polynomial equations are then chosen to determine their respective constants. From Figures 2 and 3 the respective values of $[SMM]_{t=0}$, k_1 , $[DMS]_{t=0}$, and k_2 are 5.05 μM, 0.0147 min⁻¹, 1.89 μM, and 0.0519 min⁻¹, which were similar to

the ones obtained by Mitani et al. (23). The approximations of $[SMM]_t$ and $[DMS]_t^{total}$ functions using the MacLaurin series are therefore accurate for easier determination of all the constants.

Example 2. Let us consider again Mitani et al. (23) data, this time working on a commercial scale. The kettle is a 6 m³ volume with a tubular heat exchanger area of 2.8 m² and a heat supply rate of 150 MJ·m⁻³·h⁻¹. The boiling time in this case is 80 min, and the data are reported in Table II.

Figure 4A shows that the best polynomial regression to be considered as an approximation of SMM equation is the third-order polynomial equation, while for Figure 5A, it is proven that the polynomial equation to be used is the sixth-order one for DMS. Also, from the analysis of Figures 4 and 5, the values of the constants were exhibited easily. From there, it is obtained for

$[SMM]_{t=0}$, k_1 , $[DMS]_{t=0}$, and k_2 the respective values 3.5 μM, 0.0172 min⁻¹, 1.889 μM, and 0.100 min⁻¹. These values are similar one more time to those obtained by Mitani et al. (23).

Example 3. Let us consider now our laboratory-scale boiling procedure in a 20 L insulated kettle. Different boiling conditions are applied with the same preheating protocol. The data are presented in Tables III and IV. Only one case is illustrated. The other results are following the same approach. The case to be considered in Table IV is the first column. The values of $[SMM]_{t=0}$ and k_1 are obtained using the nonlinear equation 41 and its polynomial approximation (equation 67). There are therefore obtained similar values of $[SMM]_{t=0}$ and k_1 as presented in Figures 1 and 6. The best polynomial regression in this case is the fourth-order polynomial equation. For DMS and the determination of $[DMS]_{t=0}$ and

TABLE I
Evolution of *S*-Methylmethionine (SMM) and Dimethyl Sulfide (DMS) Concentration with Time (Example 1)

Time (min)	SMM (ppb)	DMS (ppb)
0	5.05	1.77
30	3.23	1.82
60	2.07	1.84
90	1.32	1.86

TABLE II
Evolution of *S*-Methylmethionine (SMM) and Dimethyl Sulfide (DMS) Concentration with Time (Example 2)

Time (min)	SMM (ppb)	DMS (ppb)
0	3.50	1.89
30	2.06	0.49
60	1.21	0.26
80	0.85	0.18

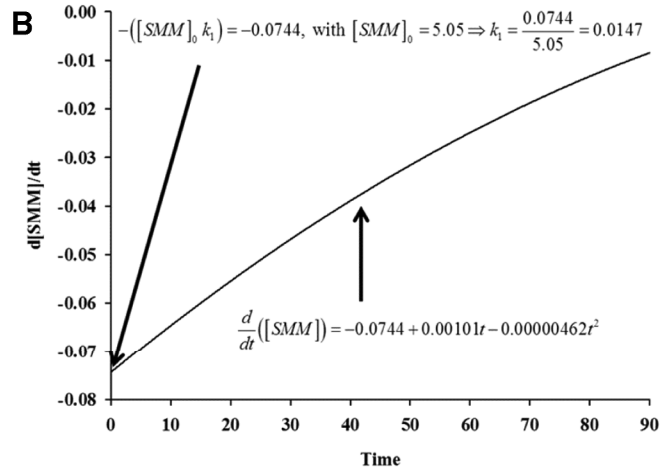
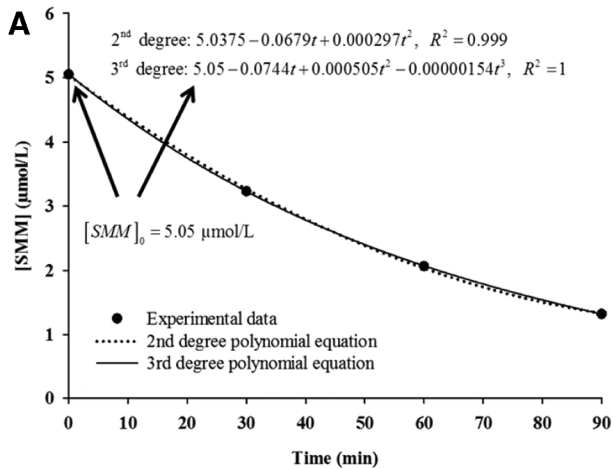


Fig. 2. A, Determination of $[SMM]_0 = [SMM]_{t=0}$ using linearized $[SMM]_t$ equation; and B, determination of k_1 using $[SMM]_t$ equation derivation (example 1).

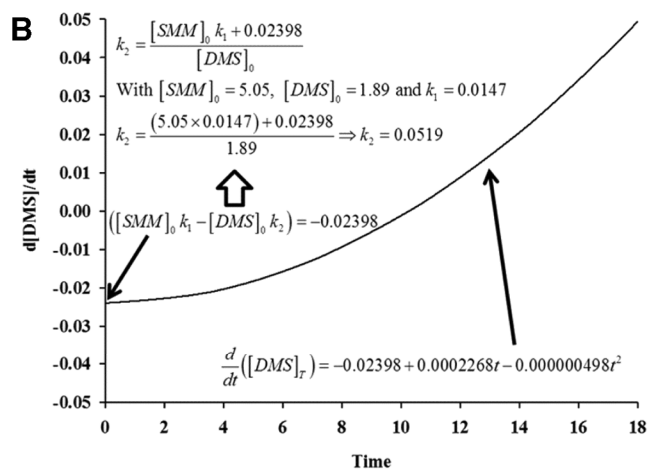
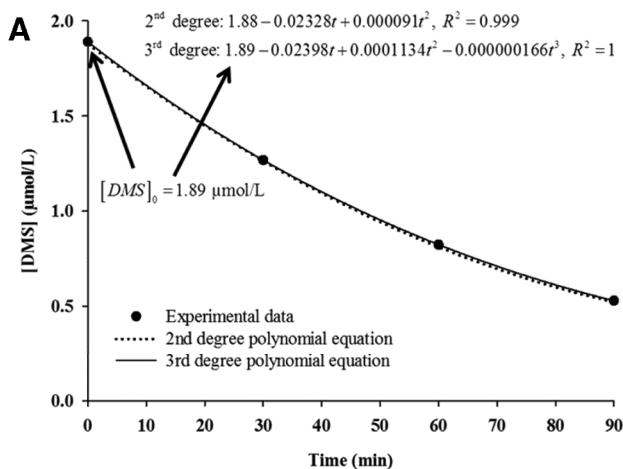


Fig. 3. A, Determination of $[DMS]_0 = [DMS]_{t=0}$ using linearized $[DMS]_t = [DMS]_t^{total}$ equation; and B, determination of k_2 using $[DMS]_t^{total}$ equation derivation (example 1).

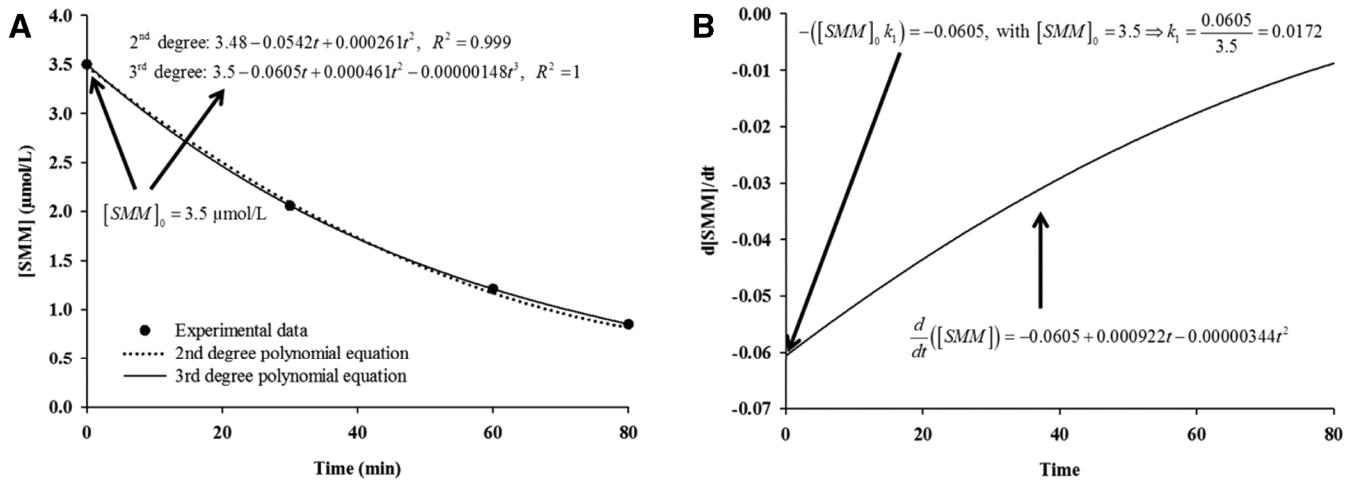


Fig. 4. A, Determination of $[SMM]_0$ using linearized $[SMM]$ equation; and B, determination of k_1 using $[SMM]$ equation derivation (example 2).

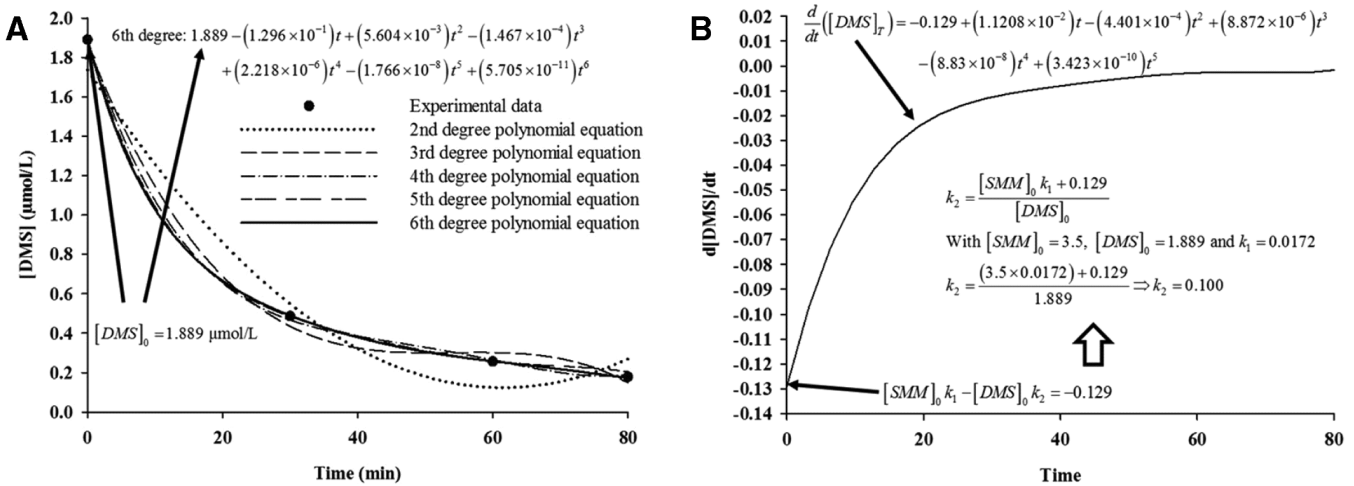


Fig. 5. A, Determination of $[DMS]_0$ using linearized $[DMS]$ equation; and B, determination of k_2 using $[DMS]$ equation derivation (example 2).

TABLE III

Comparative Evaluation of $[SMM]_0 = [SMM]_{t=0}$ and k_1 from First-Order Kinetic (Exponential) and Its Approximated Polynomial Equation (Example 3)

Time (min)	0	15	30	45	60
$[SMM]$ (ppb)	807	695.63	599.64	516.89	445.56

TABLE IV

Comparative Evaluation of $[DMS]_0 = [DMS]_{t=0}$ and k_2 from Nonlinear and Its Approximated Polynomial Equation (Example 3)

Time	1	2	3	4	5	6	7	8
Time (min)								
0	587.3	592.3	589.4	588.7	585.3	586.8	586.9	582.4
15	566.4	524.7	521.5	519.8	507.8	505.9	515.8	472.4
30	534.9	479.8	460.1	456.8	437.0	437.4	441.0	392.2
45	495.7	416.6	405.1	400.6	374.4	377.3	391.0	330.5
60	458.5	367.1	356.6	351.2	326.4	324.4	336.4	274.2
75	418.5	324.2	308.5	305.4	279.5	281.2	292.5	232.2
90	378.3	284.0	269.6	264.8	242.0	242.5	253.0	196.0
Calculated values								
$[DMS]_{0\text{ exp}}$ (ppb)	589.6	591.2	585.2	588.4	585.9	586.8	587.5	580.9
$k_{2\text{ exp}}$ (min ⁻¹)	0.01544	0.02049	0.02133	0.02165	0.02341	0.02343	0.02260	0.02751
$[DMS]_{0\text{ pol}}$ (ppb)	587.8	591.2	589.4	588.7	585.9	586.8	587.5	582.4
$k_{2\text{ pol}}$ (min ⁻¹)	0.01557	0.02046	0.02110	0.02145	0.02341	0.02341	0.02240	0.02664

(continued on next page)

^a $[DMS]_{0\text{ exp}} = [DMS]_{t=0, \text{exp}}$ and $[DMS]_{0\text{ pol}} = [DMS]_{t=0, \text{pol}}$: Initial DMS concentration obtained respectively from equation 32 and linearized polynomial equation; $k_{2\text{ exp}}$ and $k_{2\text{ pol}}$: volatilization rate coefficient obtained respectively from equation 32 and linearized polynomial equation.

k_2 , the adequate polynomial regression is the third-degree one. In this case, the calculation of these constants obtained using the linearization presented in Figure 7 is similar to the one acquired using the nonlinear function with the help of Matlab R2014a (MathWorks, Natick, MA, U.S.A.), as shown in Table IV (column 1). When analyzing Table IV for the other cases, it is therefore demonstrated that the MacLaurin series as an approximation of

nonlinear equations for SMM and DMS evolution during wort boiling is very accurate, and the determination of constants is easier.

Example 4. Let us consider the data obtained from the boiling process of two wort substitutes using a 20 L insulated kettle (13). The boiling data are presented in Table V. The approach to calculate the different constants is the same as the previous examples.

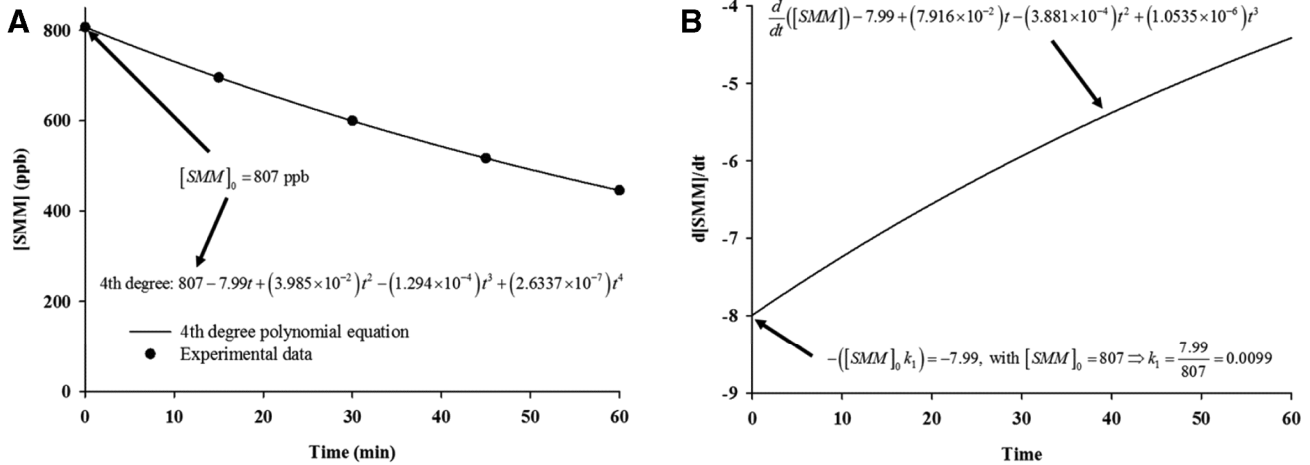


Fig. 6. A, Determination of $[SMM]_0$ using linearized $[SMM]$ equation; and B, determination of k_1 using $[SMM]$ equation derivation (example 3).

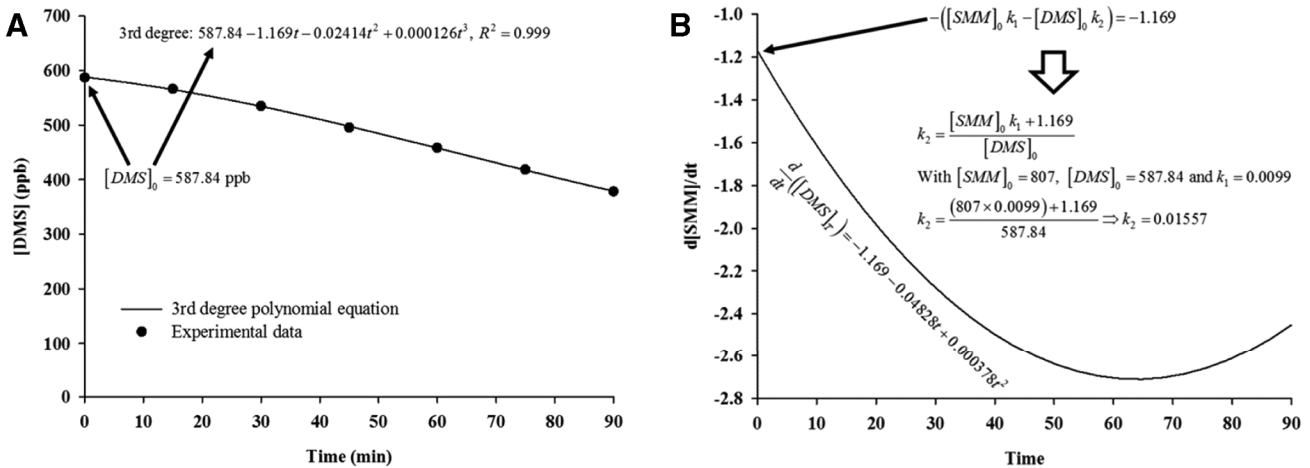


Fig. 7. A, Determination of $[DMS]_0$ using linearized $[DMS]$ equation; and B, determination of k_2 using $[DMS]$ equation derivation (example 3).

TABLE IV (continued from previous page)

9	10	11	12	13	14	15	16	17	18
584.4	585.7	586.3	587.7	586.4	589.1	587.6	586.5	586.6	586.1
463.5	454.0	443.7	433.8	392.9	320.3	306.3	291.3	261.4	243.9
380.9	360.4	341.8	333.4	286.9	193.9	184.4	176.4	144.6	129.2
311.0	290.3	274.4	256.4	213.0	137.6	125.7	119.1	95.7	88.8
257.1	242.6	219.1	212.9	160.3	102.7	96.0	90.9	74.9	69.4
216.3	199.7	198.4	182.8	133.3	83.7	78.4	73.6	60.0	55.9
182.4	166.0	165.9	151.4	109.6	69.0	66.6	61.3	52.6	47.3
583.6	584.9	586.8	587.5	586.3	589.4	587.8	585.8	586.7	586.0
0.02920	0.03118	0.03342	0.03487	0.04180	0.05842	0.06141	0.06415	0.07358	0.07882
583.9	585.6	585.8	587.5	585.6	589.1	587.6	586.4	586.6	586.1
0.02959	0.03078	0.03187	0.03386	0.04110	0.05662	0.06167	0.06461	0.07417	0.07626

TABLE V
Comparative Evaluation of $[DMS]_0 = [DMS]_{t=0}$ and k_2 from Nonlinear and Approximated Polynomial Equation at Various Power Heater Levels (Example 4)

Time	500 W		750 W		1,000 W		1,250 W		1,500 W	
	Wort 1	Wort 2	Wort 1	Wort 2	Wort 1	Wort 2	Wort 1	Wort 2	Wort 1	Wort 2
Time (min)										
0	593.00	582.00	605.00	598.00	610.00	607.00	609.00	608.00	602.00	600.00
5	536.03	541.84	537.66	545.98	530.04	540.25	512.51	519.66	484.08	501.16
10	484.54	504.45	477.82	498.49	460.57	480.84	431.31	444.16	389.26	418.61
15	437.99	469.64	424.63	455.13	400.20	427.96	362.97	379.62	313.02	349.65
20	395.91	437.23	377.37	415.54	347.74	380.90	305.46	324.46	251.70	292.05
25	357.88	407.06	335.37	379.40	302.16	339.01	257.06	277.32	202.40	243.94
30	323.50	378.98	298.04	346.40	262.55	301.73	216.33	237.03	162.76	203.76
35	292.42	352.82	264.87	316.27	228.14	268.55	182.06	202.59	130.88	170.19
40	264.33	328.48	235.39	288.76	198.24	239.02	153.21	173.15	105.24	142.16
45	238.94	305.81	209.19	263.64	172.25	212.73	128.94	147.99	84.63	118.74
50	215.98	284.71	185.90	240.71	149.67	189.34	108.51	126.49	68.05	99.18
55	195.23	265.06	165.21	219.77	130.06	168.52	91.32	108.11	54.72	82.84
60	176.48	246.77	146.82	200.66	113.01	149.98	76.85	92.40	44.00	69.20
Calculated values										
$[DMS]_{0\text{ exp}}$ (ppb)	593.00	582.00	605.00	598.00	610.00	607.00	609.00	608.00	602.00	600.00
$k_{2\text{ exp}}$ (min^{-1})	0.02020	0.01430	0.02360	0.01820	0.02810	0.02330	0.03450	0.03140	0.04360	0.03600
$[DMS]_{0\text{ pol}}$ (ppb)	592.99	582.00	604.99	597.99	609.99	606.99	608.99	607.99	601.98	599.99
$k_{2\text{ pol}}$ (min^{-1})	0.02019	0.01429	0.02359	0.01819	0.02808	0.02330	0.03447	0.03138	0.04352	0.03597

In this case, the best approximation of the nonlinear equation is obtained using the fifth-degree polynomial equation. One more time, the MacLaurin series appears to be accurate to estimate the constants $[SMM]_{t=0}$, k_1 , $[DMS]_{t=0}$, and k_2 , because the values obtained are similar to the ones obtained by Desobgo et al. in 2015 (Table V).

CONCLUSIONS

The derivation of a simultaneous DMS formation and stripping nonlinear model was described, utilizing a combination of an instantaneous mass balance and a first-order reaction equation to represent separately DMS formation and stripping. This nonlinear model was found to be identical to one proposed elsewhere in the literature by Mitani et al. (23). To facilitate the implementation of our model, linearization of our nonlinear model was conducted using a MacLaurin–Taylor series expansion. Several examples of implementation of both our nonlinear and linearized models were described.

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