Dynamic Modelling and Simulation of Cold Contact Fermentation (CCF)

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Abstract

The increased commercial presence and comparative health benefits of alcohol-free beer (AFB) provide a substantial impetus for research, particularly in the field of dynamic simulation whereby the development of accurate models can help reduce costs of experimentation. Cold Contact Fermentation (CCF) is an existing method of industrial-scale AFB production that utilises reduced fermentor temperatures and altered contact times compared to Warm Fermentation (WF), though requiring continual attention given the production of non-optimal organoleptic compositions, which drastically affect taste. In order to better understand the differences between Warm Fermentation (WF) and CCF, a DAE system is constructed based on previous WF studies whose responses are compared vis-à-vis to simulations of the same model under industrial CCF conditions. Given the significant discrepancies between dynamic results, industrial data can be for the parametrisation of a new CCF model, in order to accurately portray plant operation. Further to these simulations, the sensitivity of final species concentrations to parameter variation and the effect of hypothetical temperature profiles are studied with the aim of evaluating model system flexibility and opportunities for improvement based on changes to fermentor temperature profiles. Overall, disparate relative ethyl acetate sensitivity and clustering of hypothetical CCF responses reflect existing challenges with flavour composition but highlight opportunities for remarkable process improvements.

Keywords: Cold Contact Fermentation (CCF); Cold Contact Process (CCP); Alcohol-Free Beer (AFB); dynamic modelling; multivariate constrained dynamic optimisation.

1. Introduction

Cold Contact Fermentation (CCF) or Cold Contact Process (CCP) emerged in 1983 as novel method of producing beer with a reduced alcohol content by altering both fermentation duration and temperature from the conditions utilised in standard brewing practice (Perpète and Collin, 1999). Since that time, interest in alcohol-free beer (AFB) has surged, with an estimated global increase in consumption of 80% from 2007 to 2012 corresponding to an amount of $2.2 \cdot 10^9$ L yr^{-1} (Liguori et al., 2018). Despite this increase in consumption, the production of AFB is still beset by concerns with the issue of maintaining the balance between flavours such as butter/butterscotch (due to vicinal diketones, frequently denoted as VDKs, such as diacetyl), bitterness (due to aldehydes such as acetaldehyde) and fruitiness (due to esters, such as ethyl acetate) while retaining a consistent flavour profile with regard to sweetness (residual extract) and beer aroma.

While numerous research efforts regarding CCF at a laboratory scale have been undertaken since its inception, its dynamic modelling has not received the same attention as the produced beverage. Dynamic modelling and optimisation have been applied for

beer manufacturing (Rodman and Gerogiorgis, 2016); this work steers towards the implementation of not only a robust model but a sound platform for future optimisation on a broader industrial scale aimed at process cost reduction and flavour improvement. This study uses the kinetic model of de Andrés-Toro et al. (1998) as the basis for describing state responses under CCF conditions of suspended biomass (X_S), ethanol (C_E), sugar (C_S), diacetyl (C_{DY}) and ethyl acetate (C_{EA}) (see Fig. 1). This model splits the fermentation process into an initial lag phase and, upon adequate lag cell activation, transition to a fermentation phase where secondary flavour products are generated. The kinetic model equations (Eqs. 1–12) describing species profiles are shown in Fig. 1.

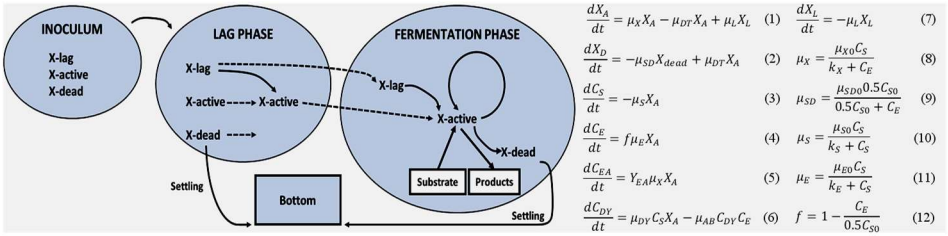

Figure 1: Kinetic model for Warm Fermentation (WF) (de Andrés-Toro et al., 1998).

Arrhenius factors (μ_i) denote formation or consumption of corresponding model species while the stoichiometric factor (Y) and inhibition factor (f) guide ethyl acetate and ethanol formation, respectively. The full mathematical model has been expressed as a Differential Algebraic Equation (DAE) system and solved in MATLAB, to simulate key responses.

2. CCF Model Parameterisation

A comparison of dynamic simulation responses for the de Andrés-Toro et al. (1998) model (T = 13 °C) and implementation of new CCF operating (T = 5–6.5 °C) and initial conditions (CCFIC) demonstrated severe differences in model dynamic behaviours, i.e., differing trends aside from the differing initial (imposed via the CCFIC) and final species concentration values (Fig. 2). Because of anticipated response discrepancies between simulations of WF and CCF in respect to assumed initial conditions, final concentrations from industrial CCF batches were incorporated as numerical benchmarks for parameterisation of de Andrés-Toro (1998) kinetic model, now under CCF conditions.

Reparameterisation of temperature-dependent parameters of specific rates (μ_i, Eq. 13) has therefore been systematically conducted, and it was achieved through an algorithm targeting least squares regression (Eq. 14) with respect to each of the state variables $\theta_{i,\text{measured}}$ (for a total of N) and corresponding model responses, $\theta_{i,\text{model}}$ (Pilarski, 2019).

$$\mu_i = \exp\left(A_i + \frac{B_i}{T}\right) \tag{13}$$

$$\min_{\theta_i} J(\theta_i) \tag{14}$$

$$J = \sum_{i=1}^{N} \left(\theta_{i,\text{measured}} - \theta_{i,\text{model}}\right)^2 \tag{15}$$

Minimisation was performed using the Nelder-Mead direct search algorithm, whereby a subset of DAE parameters were allowed to vary in order for the algorithm to converge and produce a solution set of parameters that diverged minimally from the WF parameters

presented by de Andrés-Toro et al. (1998). Plausible industrial operating conditions and/or data encompassing processing, initial conditions and final concentrations for CCF simulations and parameterisation can be considered in this computational framework.

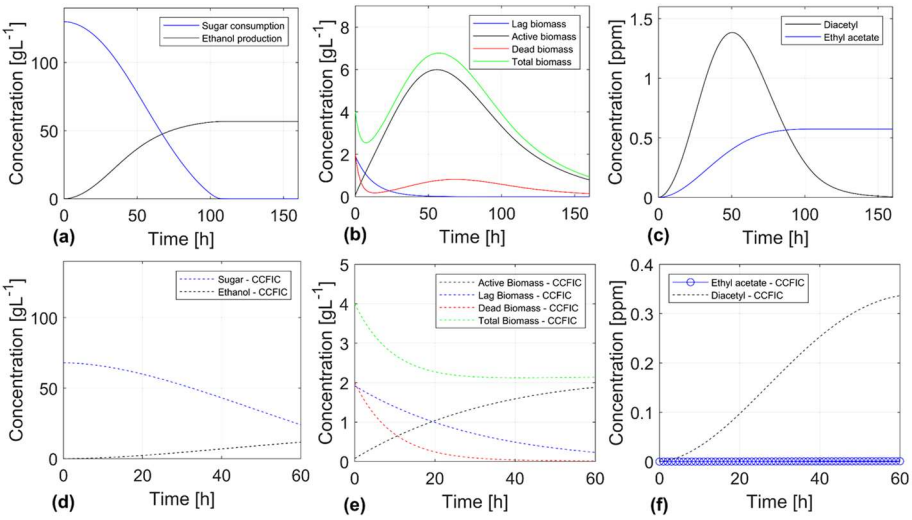

Figure 2: Key dynamic response comparisons between WF (a–c) and CCFIC (d–f).

Values of A_i and B_i for explicit kinetic model parameters which have properly converged have been then reparameterised to constrain the scope of the problem. This successfully allowed for parameterisation with respect to C_S, C_E, C_{EA} and C_{DY} based on limited pilot plant data, with all biomass responses remaining unconstrained (Fig. 3). Reparameterised CCF values, but also those kept as per the WF model, have been summarised in Table 1.

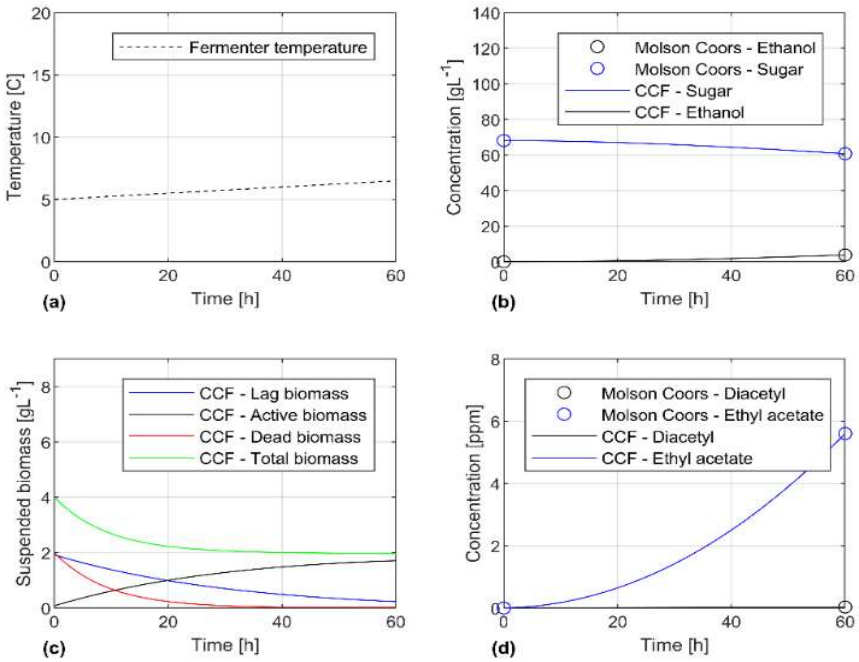

Figure 3: A plausible CCF temperature profile (a); parameterised CCF responses (b–d).

Table 1: Resulting CCF model parameters with * denoting values original to this study (our results).

Rates / Parameters	Description	A_i	B_i
μ_{SD0}	Maximum dead cell settling rate	33.820	–10,033.280
μ_{X0}	Maximum cell growth rate	37.450*	–31,934.090
μ_{S0}	Maximum sugar consumption rate	–41.920	11,754.776*
μ_{E0}	Maximum ethanol production rate	4.125*	–1,267.240
μ_{DT}	Specific cell death rate	130.160	–38,313.000
μ_{L}	Specific cell activation rate	30.720	–9,501.540
$k_E = k_S$	Affinity constant for sugar and ethanol	–119.630	35,203.709*
Y_{EA}	Stoichiometric factor - ethyl acetate production	169.130*	–26,589.000
		Value	
μ_{DY}	Rate of diacetyl production	$7.590 \cdot 10^{-6}$*	
μ_{AB}	Rate of diacetyl consumption	$1.138 \cdot 10^{-3}$	

3. Sensitivity Analysis

Sensitivity analyses offer great insight for batch and semi-batch processing that may require control policies of varying flexibility based on production progress/completion. Process response sensitivity S can be quantified in relation to the measured change in a state variable θ based on an intended change in a parameter P according to Eq. 15.

$$S = \frac{\partial\theta}{\theta} \Big/ \frac{\partial P}{P} \tag{15}$$

Parameter variations of ±5% were implemented and the resulting sensitivities of state variables (model responses) visualised for clarity (Fig. 4). Variations in parameters A_{kes} and B_{kes} produced large perturbations for all state variables, though final C_{EA} sensitivity to variation (particularly for A_{YEA}, B_{YEA}, $A_{\mu x0}$ and $B_{\mu x0}$) was most significant and a reflection of 'fruity' flavour issues described for AFB as a result of over or uncontrolled ester expression (Verstrepen et al., 2003). Thus, process variations (parameter values being a function of processing conditions) have the greatest impact on C_{EA}.

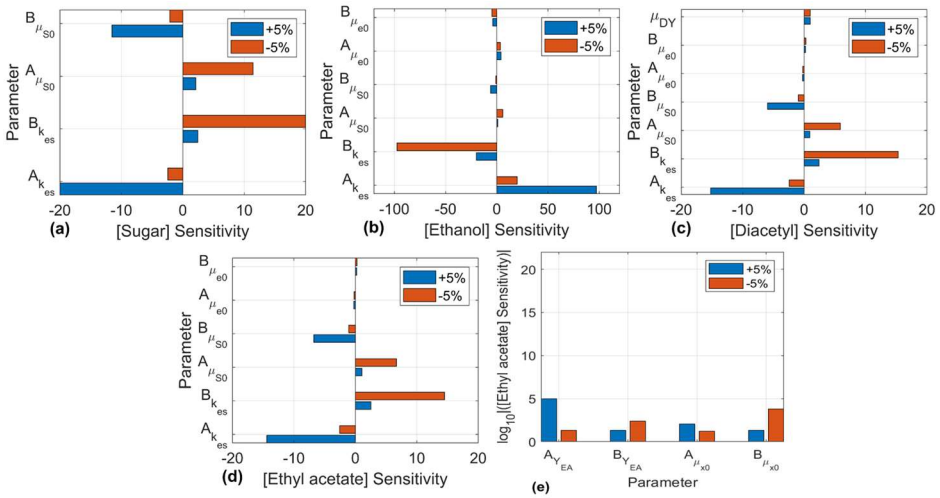

Figure 4: Sensitivities for (a) final sugar, (b) ethanol, (c) diacetyl and (d–e) ethyl acetate concentrations under ±5% variation for all parameters of non-negligible process impact.

4. Course Grid Enumeration of Hypothetical Temperature Profiles

Previous CCF industrial results were garnered via consideration of a 1.5 °C temperature band. However, it is known that CCF processes can make use of temperatures between 0–8 °C (Perpète and Collin, 1999; Montanari et al., 2009). In addition, by using existing cooling jackets, the fermentor temperature can be controlled provided the CCF progresses, through the exothermic reactions in the fermentor, or with future implementation of external heating. The effect of temperature variation was studied via coarse grid discretisation of the computational time (10 hr sub-grids for $t \in [t_0, t_f] = [0, 60]$ and temperature domains (1 °C sub-grids for 1–7 °C). Furthermore, different temperature profiles have been selected on the basis of ease of industrial implementation (Pilarski, 2019). This resulted in 29 hypothetical temperature profiles, ranked by total theoretical heat Q (Eq. 16). Here, m is the fermentation broth mass and C_P is the specific heat capacity at constant pressure. Results for all temperature profiles are given in Fig. 5.

$$Q = mC_P \int_{t_0}^{t_f} T(t)\mathrm{d}t \tag{16}$$

Of all enumerated results, C_{EA} and C_{DY} represent the largest and smallest spans of hypothetical outcomes, respectively. In addition, a general increase in consumption of final C_S and increased formation of C_E, C_{EA} and C_{DY} is noted. However, general trends for rates of change of each response are very different. When coupled with evident clustering (e.g., Trials 26–29) these trends show the potential for improvement based on changes to fermentor temperatures. Although the number of temperature profiles considered here is limited in comparison to the full scope of possibilities that could be implemented industrially, comparison of the effects of the theoretical Q limits the number of temperature profiles that allow one to stay within product specifications. Each Q may have multiple associated temperature profiles; the optimal manipulation may be established via dynamic optimisation attain target ethanol concentrations while also ensuring critical flavour component concentration constraints (Rodman et al., 2019).

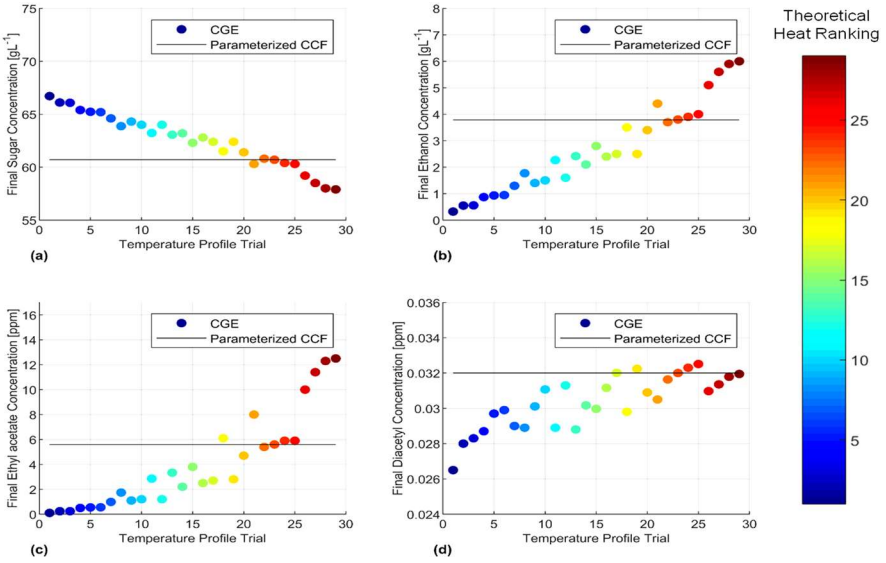

Figure 5: (a) Sugar, (b) ethanol, (c) ethyl acetate and (d) diacetyl final concentrations based on T- profile variation and ranking by a Q metric (CGE: Coarse Grid Enumeration).

5. Conclusion

This study used industrial data to formulate a newly parameterised model for CCF using the published de Andrés-Toro et al. (1998) kinetic model to compare model responses between WF and CCF. Differences in dynamic behaviour, aside from different initial and final species concentration values inherent of the different processing requirements of WF and CCF operations, necessitated reparameterisation of the Andrés-Toro model to accurately describe CCF. Subsequent parameterisation regarding industrial data points provided a solution set of parameters to follow the dynamic behaviour of the WF model. Sensitivity analyses based on a ±5% variation elucidated the most important model parameters with the highest sensitivity to changes in temperature-dependence, with ethyl acetate concentrations being the most impacted. Enumeration of CCF responses based on hypothetical temperature profiles confirmed that increased theoretical heat increased formation of ethanol, ethyl acetate and diacetyl during CCF, albeit at different rates. Future work will implement the newly parameterised CCF model for dynamic optimisation of temperature profiles in order for low-alcohol content beer subject to different end-point (related to flavour species) and interior-point (related to temperature boundaries and gradient limitations associated with controllers) constraints as well as heat transfer dynamics to account for different scales of fermentor operation and production.

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