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A kinetic model for beer production under industrial operational conditions

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Abstract

A kinetic model for beer production is proposed. The model takes into account five responses: biomass, sugar, ethanol, diacetyl and ethyl acetate. In contrast with previously published models, this model segregates biomass into three components: lag, active and dead cells and considers the active cells as the only fermentation agent. Experiments were first performed at laboratory scale and isothermal runs were carried out at five temperatures (8°C, 12°C, 16°C, 20°C and 24°C). Fitting of experimental data was made by non-linear regression. Parameter values calculated were similar to those given in the literature. The kinetic model was able to fit experimental data with a very good agreement. Afterwards, experiments were conducted at pilot plant scale and runs were now carried out changing temperature with time, in the industrial way. The kinetic model, with the parameter values calculated as a function of temperature, was able to predict with a very high accuracy the non-isothermal experimental data achieved. This model can be used for simulation of the industrial process under different operational conditions and for faults detection. It can also be utilized for the optimization and even for the supervised control of the process and its automatization. © 1998 IMACS/Elsevier Science B.V.

Keywords: Kinetic model; Beer fermentation; Bioprocess modelling

1. Introduction

The conventional industrial production of beer is based on a batch fermentation of wort, with no stirring. A temperature profile along fermentation time is applied in order to obtain the required ethanol level, and the desired properties (such as taste, aroma, etc.).

Mathematical models of wort fermentation have been developed to simulate the industrial process in order to carry out the optimization of operational conditions and even for process control. Some of these models have been developed from laboratory data [1–4], other models describing only partially the process [5,6], not always taking into account important factors affecting beer quality [6], and some

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being structured, very complex and not useful for control or optimization purposes [7].

The aim of this work has been to develop a model for industrial use, having in view the following purposes:

- The optimization of the process.
- The detection of process deviations or faults.
- The development of software sensors.

Temperature is the only manipulated variable during beer fermentation. So it is important to model the temperature effects on the process dynamics.

The experimental data have been first obtained carrying out batch fermentations, without stirring, at constant temperature, using industrial wort and yeasts supplied by Cruzcampo Breweries (Madrid, Spain). Afterwards, in order to check the model, data have been achieved at pilot plant scale, the runs now being conducted with a temperature profile (in a similar way to that employed in industrial fermentation processes of breweries). Since no mechanical stirring is applied, the model has to consider sedimentation of biomass.

Once obtained, the model has been used to get an optimal temperature profile. Dynamic programming and genetic algorithms were applied. This second method furnished a fast and simple way to calculate a fine discretization of the optimal profile. Moreover, the model has been used for fault detection, during the computer-based real-time control of the pilot plant.

2. Kinetic model

The kinetic model proposed takes into account five responses: biomass (X), substrate (C_s), ethanol (C_e), diacetyl (C_{dy}) and ethyl acetate (C_{ea}).

2.1. Modelling biomass evolution

Biomass is segregated into three different types of cells: lag (X_{lag}), active (X_{act}) and dead (X_{dea}) cells. The biomass behaviour is shown in Fig. 1. We have experimentally determined that the whole process can be divided into two consecutive phases: a lag phase and a fermentation phase. At the beginning, when the activation process starts, no fermentation is observed. Thus, it is possible to define a lag phase in which only two processes can be observed: dead cells are settling down to the bottom and lag cells are being activated. When about 80% of lag cells have been transformed into active cells, fermentation and growth start, beginning the fermentation phase. From this moment these last two processes, together with settling and activation processes, already active in the lag phase, take place simultaneously. The time at which the lag phase ends and the fermentation phase begin has been named t_{lag}.

The proportion of each type of cells was determined experimentally. As a relatively old inoculum was used, the proportion of dead cells was higher than those usually found in breweries but the model can be applied to any cell type distribution. In our case, it is assumed that inoculum (X_{inc}) is composed of about 50% of dead cells, 48% of lag cells and only 2% of active cells

$$X_{act}(0) + X_{lag}(0) = 0.5 \cdot X_{inc}(0), \quad t < t_{lag} \tag{1}$$

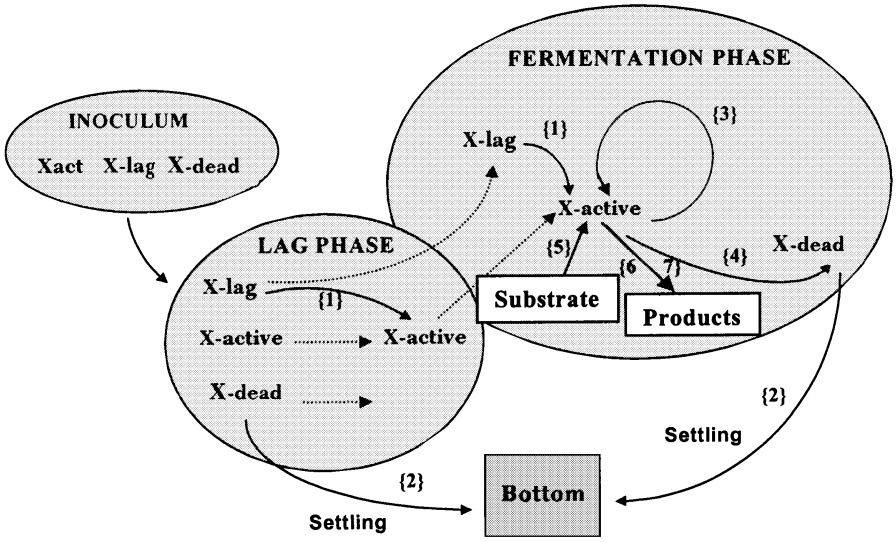

Fig. 1. Process scheme considered in the kinetic model.

Immediately after inoculation, all the yeast become suspended in the wort (X_{sus}), that is

$$X_{sus}(t) = X_{act}(t) + X_{lag}(t) + X_{dea}(t) \tag{2}$$

and the dead yeast are settling down with a rate μ_{SD} (reaction 2 in Fig. 1) decreasing the suspended cells, according to

$$\frac{dX_{sus}(t)}{dt} = -\mu_{SD} \cdot X_{DT}(t) = -\mu_{SD}(X_{sus}(t) - 0.5 \cdot X_{inc}), \quad t < t_{lag} \tag{3}$$

Experimental data showed that μ_{SD} depends on the density of the wort (proportional to the initial substrate concentration, C_{s_0}), and on CO_2 production that avoids settling. CO_2 concentration has been measured as ethanol concentration (C_e). μ_{SD_0} is the maximum value that can be reached; in this case it is attained at the beginning of the process. Then

$$\mu_{SD} = \frac{\mu_{SD_0} \cdot 0.5 \cdot C_{s_0}}{0.5 \cdot C_{s_0} + C_e(t)} \tag{4}$$

Also the lag yeasts became active (reaction 1 in Fig. 1) with a rate given by

$$\frac{dX_{act}(t)}{dt} = \mu_{lag} \cdot X_{lag}(t) = \mu_L(0.5 \cdot X_{inc} - X_{act}(t)), \quad t < t_{lag} \tag{5}$$

in which μ_L is the specific rate of activation.

During the fermentation phase, active yeasts grow, producing new biomass (reaction 3 in Fig. 1) with a rate given by the first term in Eq. (6). Part of them die (reaction 4 in Fig. 1), with a rate given by the second term of Eq. (6), and also the remaining lag yeasts continue their activation with the rate given by the third term of the same equation. Thus, the increase in active yeasts can be described as follows:

$$\frac{dX_{act}(t)}{dt} = \mu_x \cdot X_{act}(t) - \mu_{DT} \cdot X_{act}(t) + \mu_L \cdot X_{lag}(t), \quad t > t_{lag} \tag{6}$$

In this equation, μ_x, the specific rate of growth, can be substituted by an empirical relationship of this variable with the substrate and ethanol concentrations, according to

$$\mu_x = \frac{\mu_{x_0} \cdot C_s(t)}{k_x + C_e(t)} \tag{7}$$

in which μ_{x_0} is the maximum specific growth rate.

2.2. Modelling substrate consumption

The rate of sugar consumption has been considered to be given by

$$\frac{dC_s(t)}{dt} = -\mu_s \cdot X_{act}(t) \tag{8}$$

where μ_s, the specific substrate consumption rate, has been assumed to be a Michaelis–Menten function of the substrate concentration, according to

$$\mu_s = \frac{\mu_{s_0} \cdot C_s(t)}{k_s + C_s(t)} \tag{9}$$

in which μ_{s_0} is the maximum specific consumption rate, reached at substrate saturation, which in this case occurs at the initial concentration of sugar (s_0), and k_s is an affinity constant.

2.3. Modelling product and by-products synthesis

Ethanol production rate has been described as a function of the active biomass

$$\frac{dC_e(t)}{dt} = \mu_e \cdot X_{act}(t) \tag{10}$$

Experimental work showed that ethanol concentration did not vary in a monotonous way during the fermentation time, but showed a decreasing rate with time. To include this inhibition effect in the model, one inhibition factor, f, of the specific rate of ethanol production, μ_e has been taken into account. This factor, f, has been made proportional to the maximum amount of ethanol that can be produced, i.e. half the initial sugar concentration. Thus the following equation can be employed:

$$\frac{dC_e(t)}{dt} = f \cdot \mu_e \cdot X_{act}(t) \tag{11}$$

where

$$f = 1 - \frac{C_e(t)}{0.5 \cdot C_{s_0}} \quad \text{and} \quad \mu_e = \frac{\mu_{e_0} \cdot C_s(t)}{k_e + C_s(t)} \tag{12}$$

The by-product production rates, diacetyl (C_{dy}) and ethyl acetate (C_{ea}), were also taken into account. Ethyl acetate concentration changed as predicted by Gee and Ramirez [4], with a constant stoichiometric coefficient acetate/sugar, Y_{eas}, according to

$$\frac{dC_{ea}(t)}{dt} = Y_{eas}\frac{dC_s(t)}{dt} \tag{13}$$

Diacetyl concentration evolution is much more complex. This compound is produced mainly during the first hours of fermentation process, but a part is converted afterwards into acetoin and 2,3-butanediol. Therefore, the diacetyl production rate must take into account both processes; one of them is the appearance rate, taken as proportional to the sugar concentration, the other process is the reduction or disappearance, assumed to be proportional to ethanol concentration, as indicated by the following equation:

$$\frac{dC_{dy}(t)}{dt} = \mu_{dy} \cdot C_s(t) \cdot X_{act}(t) - \mu_{ab} \cdot C_{dy}(t) \cdot C_e(t) \tag{14}$$

2.4. Temperature dependence

According to the above description, the model has 10 parameters, including nine specific constants of production and consumption rates and one Michaelis type constant. Most of them have been assumed to be affected by the temperature. These relationships can be described by exponential equations of the Arrhenius type, as

$$\mu = A\exp(B/RT) \tag{15}$$

3. Experimental

3.1. Experimental set-up

Two experimental set-ups have been employed.

One of the set-ups has been built for the isothermal batch fermentations, under computer monitoring and control (as can be seen in Fig. 2). In each experiment a set of 3 l vessels without stirring, filled up to 2.5 l with wort and inoculated with a yeast suspension (1:100 v/v) was used. Five temperatures were assayed (8°C, 12°C, 16°C, 20°C and 24°C). Runs were replicated three times to improve the accuracy of the experimental data. Biomass, substrate and ethanol concentrations together with pH were measured with time. In addition, an experimental series was dedicated to study the evolution of the concentrations of suspended and total biomass along fermentation, for the five temperatures.

Experiments have also been carried out in a pilot plant scale. A scheme of the pilot plant is shown in Fig. 3. The fermenter, of 100 l in volume, was filled with 80 l of wort, inoculated with yeast (1:100 v/v). The fermentation proceeded following the industrial temperature profile of Fig. 4. By means of interface electronics, a computer was used for data acquisition from the sensors, and for temperature control.

An intelligent environment, called Kappa-PC (from Intellicorp) was adapted for the real-time monitoring and control work, including fault detection features based on the simulation of the process (with the new model).

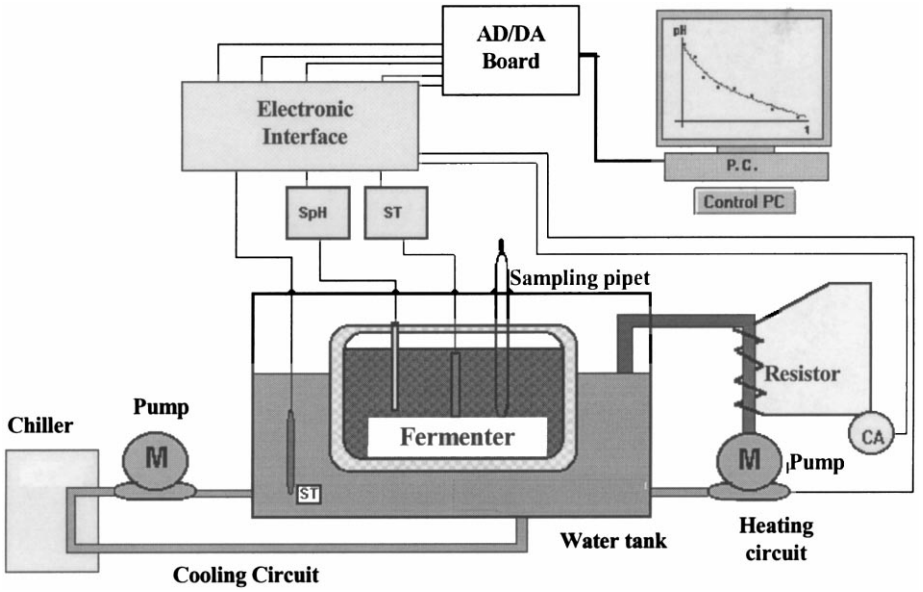

Fig. 2. Experimental set-up for the isothermal studies.

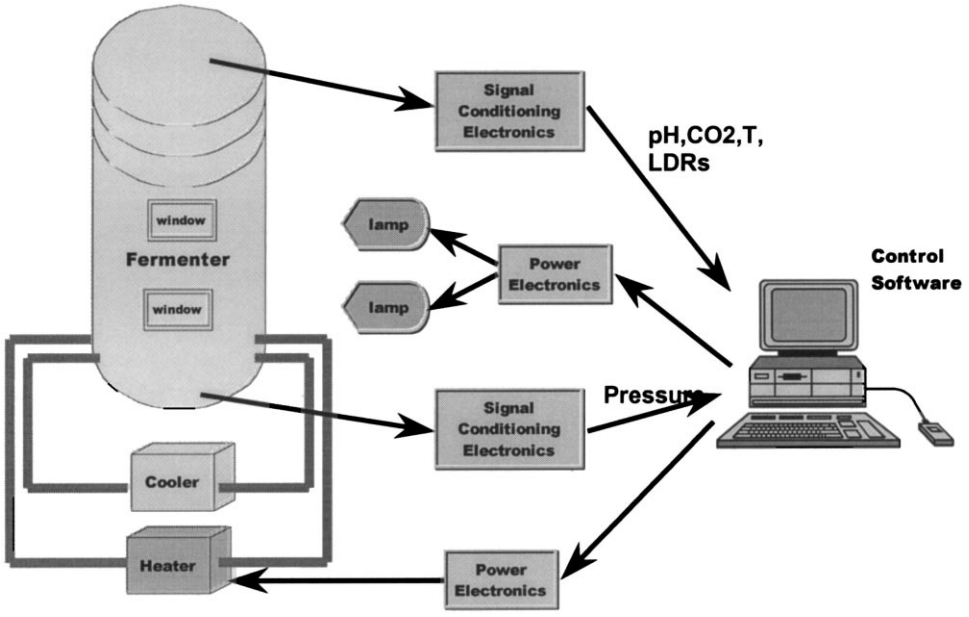

Fig. 3. Pilot plant set-up.

Suspended biomass was measured on line by the increase in absorbance detected by a photocell placed in the middle of the vessel. It was also measured out line by dry weight. Ethanol concentration was also estimated on line by the decrease of hydrostatic pressure measured by a pressure sensor at the bottom of the vessel. Five runs were carried out at this scale.

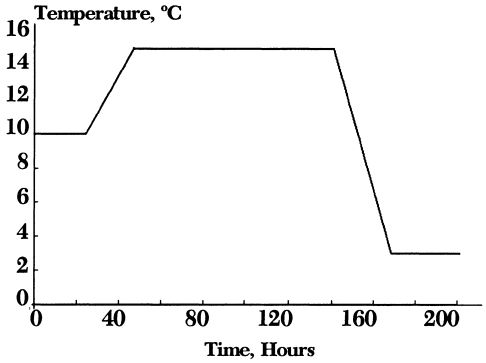

Fig. 4. Industrial temperature profile.

3.2. Analytical methods

Total sugars were determined by HPLC. Ethanol by the Scaba method (in the industrial brewery). Diacetyl was calculated from previously published data [2].

The fitting of the experimental data to the proposed model was carried out by multi-response non-linear regression algorithm, coupled with a numerical integration routine, because integral data were being analysed.

4. Results and discussion

4.1. Parameter values determination

According to the method quoted above, the values of the parameters were calculated, which are shown in Table 1. In this table the functions of the temperature finally adopted are also given. These values are, in general, of the same order of magnitude of those previously reported for beer fermentation at laboratory scale [4].

Fig. 5 shows the fitting of the model to the experimental data, corresponding to one fermentation at constant temperature, 12°C. At the other four tested temperatures, similar good fittings were obtained, showing the good predictive performance of the model.

4.2. Validation of the model

The kinetic model, with the parameter values achieved by fitting of isothermal data, was used to predict the experimental results of non-isothermal experimental data, taking into account biomass, substrate and product concentration evolution. These runs were performed at pilot plant scale, under a temperature profile shown in Fig. 4. Again the prediction of the model was very good, as can be observed in Fig. 6.

Table 1
Parameter values calculated by fitting experimental data as functions of temperature

μ_{x_0}=exp(108.31−31934.09/T)
Y_{eas}=exp(89.92−26 589/T)
μ_{s_0}=exp(−41.92+11654.64/T)
μ_{lag}=exp(30.72−9501.54/T)
$\mu_{dy}=-6.1344\times10^{-8}\cdot T^2+8.4266\times10^{-6}\cdot T-1.7672\times10^{-2}$
$\mu_{ab}=-9.1384\times10^{-7}\cdot T^2+6.7071\times10^{-5}\cdot T-0.1251\times10^{-3}$
μ_{DT}=exp(130.16−38 313/T)
μ_{SD_0}=exp(33.82−10033.28/T)
μ_{e_0}=exp(3.27−1267.24/T)
k_e=exp(−119.63+34203.95/T)

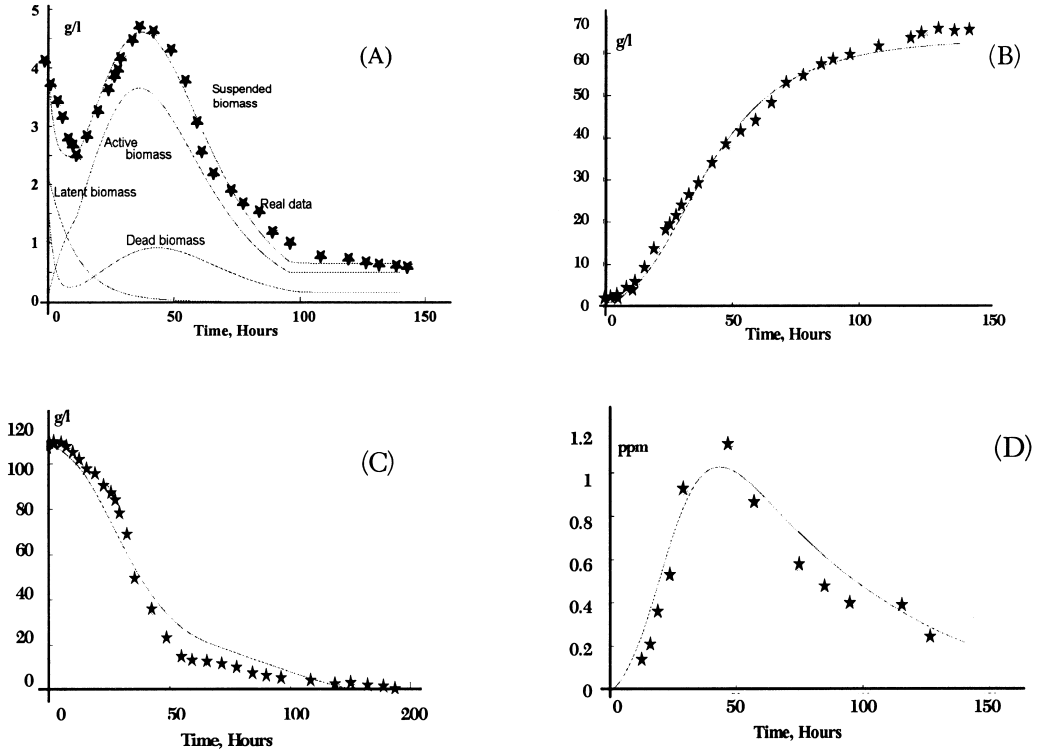

Fig. 5. Time courses of the concentrations of (A) biomass, (B) ethanol, (C) total sugars, and (D) diacetyl. Stars: experimental points. Solid line: model prediction.

5. Conclusions

As demonstrated by the experimental results, the model seems to be adequate to perform simulations of the industrial batch beer fermentation. The model is useful to study the process behaviour under different operational conditions, in order to process optimization. Also the model can be useful to

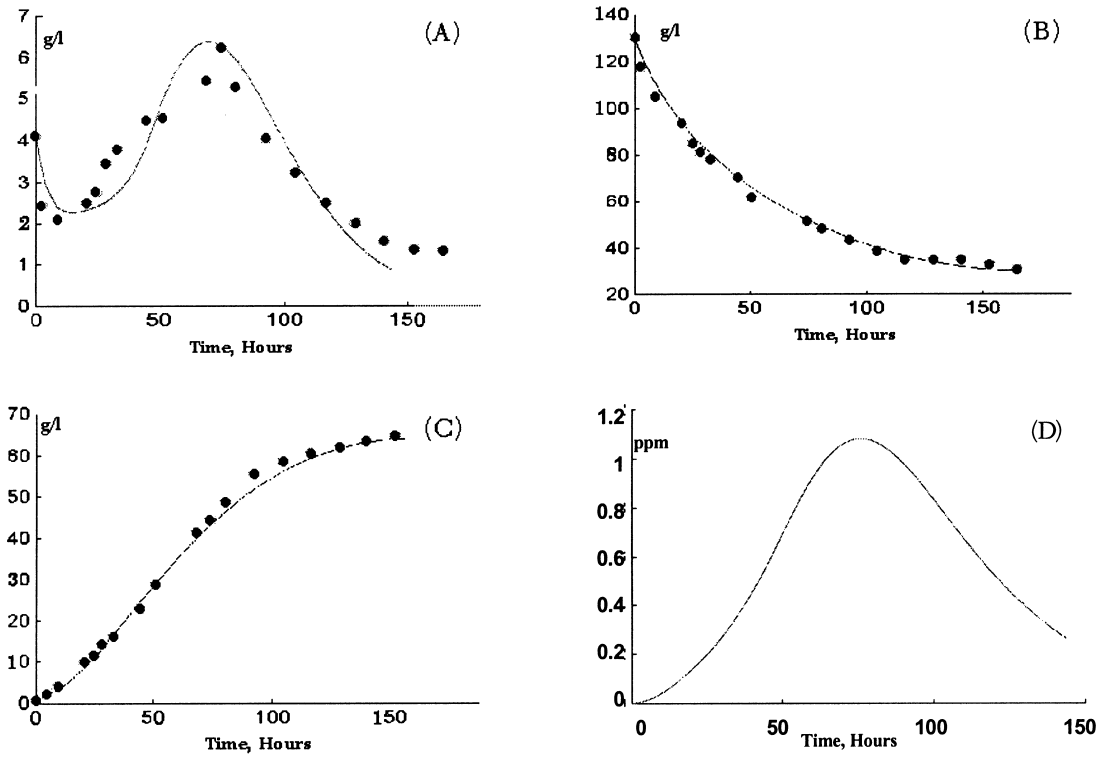

Fig. 6. Time courses of the concentration of (A) biomass, (B) total sugars, (C) ethanol and (D) diacetyl. Circles: experimental data obtained in the pilot plant run with the temperature profile of Fig. 4. Line: prediction of the model with the parameters calculated from the isothermal experiments.

implement software sensors and model-based control techniques such as internal model control schemes, and fault diagnosis for autonomous operation.

Future work is the consideration of economic and technological aspects of the optimal temperature profiles. That means the extension of the model to consider thermodynamic factors.

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