MODEL-BASED OPTIMIZATION OF THE OPERATION PROCEDURE OF AN EMULSIFICATION PROCESS

M. Stork and O. H. Bosgra
Mechanical Engineering Systems and Control Group
Delft Universtity of Technology
Mekelweg 2, 2628 CD Delft

J. A. Wieringa and A. J. Krijgsman
Unilever Research Laboratorium Vlaardingen
Olivier van Noortlaan 120, 3130 AC Vlaardingen

Abstract

This work addresses the model-based optimization of the operation procedure of an emulsification process using a stirred vessel in combination with a colloid mill and a recycle. The computation of input trajectories (i.e. the stirrer and rotor speed in time), for reaching a certain predefined drop size distribution in minimal time, is studied. It is argued that gradient based optimization techniques do not give satisfactorily results for this optimization problem. In Stork et al. (2002) the optimization of an emulsification process using a stirred vessel only is studied. In the suggested approach the original minimum time problem is approximated as a Mixed Integer Linear Program (MILP). The solution of the MILP is a good solution of the original optimization problem. In this work this approach is extended to the optimization of the operation procedure of the total system. An optimization study shows the feasibility of the approach and it illustrates the benefit of using model-based optimization for improving the operation procedure of emulsification.

Keywords

Emulsification, Optimization, MILP, Drop size distribution.

1. Introduction

Emulsification is an essential manufacturing technology in the food industry. Examples of emulsions[1] are mayonnaise and dressings. Equipment as used for the production of oil-in-water (o/w) emulsions is shown in Figure 1. It consists of a stirred vessel in combination with a colloid mill and a recirculation loop. The vessel is equipped with a scraper stirrer: a device that consists of several blades rotating at low speed at a small distance from the vessel wall in order to achieve mixing and breaking of the oil drops. The colloid mill consists of a stator and a rotor. In the narrow gap between these the intensity of the hydrodynamic forces acting on the drops is very high, which causes the breakage of the oil drops. The colloid mill also acts like a pump resulting in a recirculating flow to the vessel. The process is operated fed-batch wise and typical production times are in the order of several minutes.

Currently the operation procedure is conventional in the sense that the oil flow addition rate and the stirrer and rotor speed are set to constant values in time. After the oil addition the process is continued for a specified amount of

[1] An emulsion is a dispersion of one liquid in another one with which it is incompletely miscible.

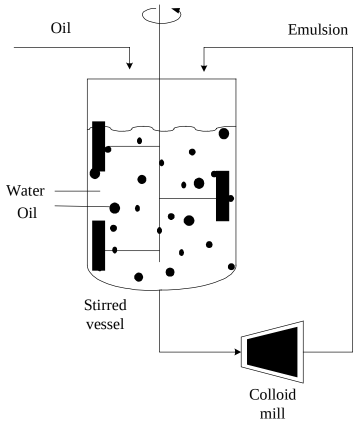

Figure 1. Equipment for the production of o/w-emulsions.

time to ensure a sufficient drop size reduction. For profit maximization it is desirable to decrease the production time while maintaining the product quality specifications. Experiments are time-consuming and expensive; because of this a model-based approach is followed in this work. The emulsion quality is strongly affected by the drop size distribution (DSD). The desired DSD is often multi-modal and/or asymmetric. This makes the control of the moments of the DSD inadequate and necessitates the control of the full distribution. One possible control configuration is as follows: first an off-line optimization problem is solved to calculate the input variables as function of the time such that a certain predefined DSD is reached in minimal time. After that a controller is designed for the tracking of the computed optimal DSD trajectory. In this paper the off-line optimization problem is studied. To the authors knowledge this is not addressed in the literature. It was found that gradient based optimization techniques do not give satisfactorily results for the solution of this optimization problem. In Stork et al. (2002) the computation of stirrer profiles for reaching a certain predefined DSD in minimal time in the stirred vessel is studied. Due to the specific model structure and by using results of Bemporad and Morari (1999) they were able to approximate the original minimum time problem as a Mixed Integer Linear Program (MILP). The solution of the MILP is a good solution of the original optimization problem. In this work this approach is extended to the optimization of the operation procedure of the total system.

The structure of this paper is as follows. A short description of the model is given in Section 2. In Section 3 the optimization problem is presented and it is explained that gradient based optimization techniques do not give satisfactorily results for the solution of it. The MILP approach is presented in Section 4 and in Section 5 the results of an optimization study are presented. Finally, concluding remarks are stated in Section 6.

2. Outline of the model

The hydrodynamic forces that are generated by the stirrer and the rotor cause the breakage of oil drops and because of this the DSD changes in time. The model describes the DSD(t) and it consists of two parts: a Reactor model and a Drop model. The Reactor model describes the phenomena occurring at macro-scale. It describes the drop movement and the local hydrodynamical conditions, which are acting on the drops as function of the equipment design and the stirrer and rotor speed. The Reactor model consists of four compartments and for each compartment a population balance equation PBE (Ramkrishna, 2000) is formulated to describe the DSD(t). It is assumed that coalescence is negligible and that breakage occurs in a small region round the stirrer and in the colloid mill. This is modeled with three compartments: one describing the breakage round the stirrer (the Laminar compartment), one for the bulk volume of the vessel (the Bulk compartment) and the third for the breakage in the colloid mill (the Colloid mill compartment). The fourth compartment describes the DSD(t) in the piping (the Pipe compartment).
The Drop model describes the phenomena occurring at the drop level. It describes the breakage condition, the breakup time and the number and sizes of the daughter drops. These relations are based on theory as currently available regarding drop breakage (see for example Grace, 1982 and Wieringa et al., 1996). The model is not yet validated.

3. Formulation and features of the optimization problem

We want to chose the stirrer speed, the oil flow addition rate and the rotor speed as a function of the time such that a certain predefined DSD is reached in minimal time. Gradient based optimization techniques do not give satisfactorily results for this optimization problem because the breakage phenomena depend in a strong nonlinear fashion on the stirrer and rotor speed. A very small increase of the stirrer/rotor speed may already lead to the breakage of certain drop sizes that would not break with a slightly lower value of the stirrer speed. Comparable behavior is observed for the formation of certain drop sizes; until some stirrer/rotor speed they are not formed whereas they are formed rapidly at a stirrer/rotor speed that is only slightly higher. A further increase of the stirrer/rotor speed may suddenly lead to the non-formation or even breakage of these drop sizes. Gradient based optimization methods do not give satisfactorily results because of this behavior. Also non-gradient based methods like genetic algorithms do not guarantee satisfactorily behavior. Global optimality can not be guaranteed and it is unsure if even a feasible solution will be obtained.

4. MILP approach

In Stork et al. (2002) an approach is suggested that approximates the original nonlinear optimization problem as a MILP. It is explained that the strong nonlinearity is only in the dependence of the stirrer speed. Further, in small intervals of the stirrer speed (the *modes* of the system) the dynamics are linear if the stirrer speed is fixed at a constant value. This insight, together with the results of Bemporad en Morari (1999), enables to approximate the original optimization problem as a MILP. Before the mathematical formulation of the optimization problem as a MILP is given we mention that, for the optimization problem under consideration, the modes are combinatorial in itself. For example, if the number of modes with respect to the stirrer speed equals 5 and with respect to the rotor speed equals 30, then the total number of modes is 150. Further is should be mentioned that the oil flow addition rate is not considered as an optimization variable. If it is included in the optimization problem we end-up with a Mixed Integer Nonlinear Program (MINLP) which is undesirable, because they are generally hard to solve. This is why for the moment only the stirrer and rotor speed are considered. Next, the mathematical formulation of the MILP is presented.

4.1 System behavior

A set of periods (k=1,…,N) of fixed duration is defined. The following binary variable is introduced to characterize the system behavior:

$$\delta_k^s = \begin{cases} 1 & \text{if the system is in mode } s \text{ over period } k \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

The system can be in only one mode at a point in time. This is expressed mathematically as $\sum_{s=1}^{n_s} \delta_k^s = 1$, with n_s the number of modes of the system. For the ease of implementation discrete time domain models are used. For each mode s we have the discrete time model:

$$x_{k+1} = A_k^s x_k + B_k^s \tag{2}$$

The states x_k are the number of drops, with a certain volume, in the Laminar, the Bulk, the Colloid mill and the Pipe compartment. While the system is in mode s, the corresponding equations characterizing the behavior of the system must hold in that mode. A new continuous variable z_k^s is defined and with linear equality and inequality constraints it is enforced that this variable is equal to x_k as the system is in mode s and that it is zero as this is not the case. Mathematically:

$$x_{k+1} = \sum_{s=1}^{n_s} (A_k^s z_k^s + B_k^s \delta_k^s) \tag{3}$$

$$\sum_{s=1}^{n_s} z_k^s = x_k \tag{4}$$

$$z_k^s \le P \delta_k^s \tag{5}$$

$$z_k^s \ge 0 \tag{6}$$

With P being a weighting matrix; it must be chosen such that Eq. (5) can always be satisfied. Hence, if δ_k^s is zero then z_k^s is zero. Since δ_k^s is one for only one mode, $z_k^s = x_k$ for that mode.

4.2 End-point inequality constraints and the objective function

We now turn our attention to handling the inequality end-point constraints and the formulation of the objective function J. The following binary variable is introduced to characterize the inequality end-point constraints:

$$Y_k = \begin{cases} 1 & \text{if the inequality end-point constraints} \\ & \text{are met over period } k \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

The constraints are now expressed as:

$$Y_k x_{\min} - x_k \le 0 \tag{8}$$

$$x_k - x_{\max} - (1 - Y_k) Q \le 0 \tag{9}$$

With Q being a weighting matrix; it must be chosen such that Eq. (9) can always be satisfied. Hence, if x_k is less than its lower bound $x_{\min}$ then Y_k must be zero in order to satisfy inequality constraint (9). If x_k is larger than its upper bound $x_{\max}$ then Y_k is also set to zero. Y_k can be either one or zero if the bounds are met. Due to the formulation of the objective function J, Y_k will be set to one. The objective function is written as:

$$\max J = \sum_{k=1}^{N} Y_k \tag{10}$$

This way the number of periods, where the end-point constraints are satisfied, are maximized. Hence, the time needed to satisfy these constraints is minimized. Note, that once the constraints are met, they can be kept feasible by switching off the stirrer and the colloid mill.

5. Optimization of the operation procedure

Here the results of an optimization study are presented. The discretized model consists of 52 states (13 for each compartment). The states of the Bulk compartment are denoted as x_1 till x_{13} (x_1 correspond to the smallest drops whereas x_{13} corresponds to the largest drops). The target DSD, which is chosen for illustrative purposes only, is now defined as follows: $x_2 \geq 0.159$ (drop diameter of 2.5 micrometer) and the values of the states corresponding with drop diameters of 10 till 500 micrometer must be between 0 and 1.10^{-3} (x_5 till x_{13}). These constraints are met after 108 s if the stirrer and rotor speed are set to constant values in time (0.4 s^{-1} and 41.5 s^{-1} respectively) and if the oil flow addition rate is chosen such that the oil is added in 12 s. The stirrer and the rotor speed are allowed to vary between 0 and 0.5 s^{-1} and 0 and 100 s^{-1} respectively. A sample interval of 12 s is used for the derivation of the discrete time domain models and the time horizon is set to 108 s. Hence, 9 control moves are allowed. The system has 3 modes with respect to the stirrer speed and 32 modes with respect to the rotor speed. So, the total number of modes is 96. This implies that the MILP consists of 874 (9*96+10) binary variables and tens of thousands inequality constraints. The MILP is solved using GAMS/CPLEX.

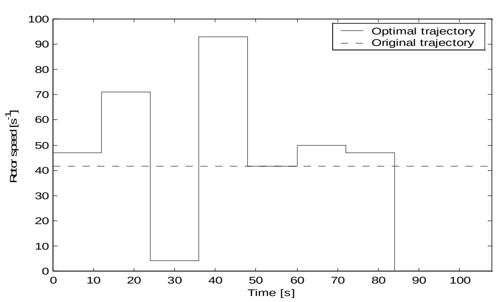

Figure 2. Optimal and original rotor speed trajectory.

The global optimum of the MILP is found after 831 nodes (2.5 hours). It is found that the constraints are met after 84 s: a decrease of the production time with 22%. The optimal stirrer and rotor speed trajectories are shown in Figure 2 and 3 respectively together with the original trajectories. The corresponding DSD's in the Bulk compartment are shown in Figure 4.

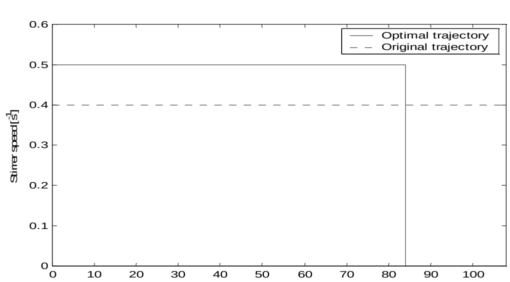

Figure 3. Optimal and original stirrer speed trajectory.

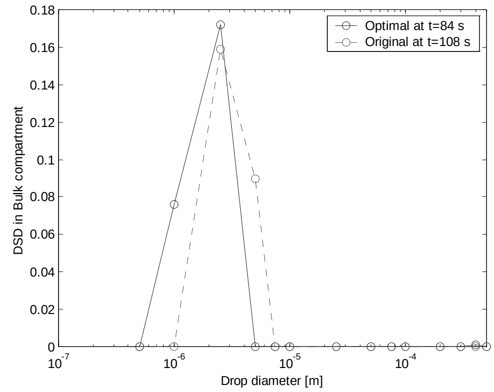

Figure 4. Optimal and original DSD in the Bulk compartment.

These results suggest that the operation procedure of an emulsification process can be improved by using time-varying stirrer and rotor speed trajectories, which is in contrast with common industrial practice.

6. Conclusions

In this work the optimization of the operation procedure of an emulsification process is studied. The suggested approach enables the computation of stirrer and rotor speed trajectories for reaching a certain predefined DSD in minimal time. An optimization study shows the feasibility of the approach and the results suggest that the operation procedure can improved by using time-varying stirrer and rotor speed trajectories, which is in contrast with common industrial practice. In order to establish what improvements can be reached the quality of the model has to be established; this is subject of current research.

References

Bemporad, A. and Morari, M. (1999). Control of systems integrating logics, dynamics and constraints. *Automatica*, 35: 407-427.

Grace, H. P. (1982). Dispersion phenomena in high viscosity immiscible fluid systems and application of static mixers as dispersion devices in such systems. *Chem. Eng. Commun.*, 14: 225-277.

Ramkrishna, D. (2000). Theory and applications to particulate systems in engineering. *Academic Press*, San Diego.

Stork, M., Tousain, R. L. and Bosgra, O. H. (2002) A MILP approach to the optimization of the operation policy of an emulsification process. *Comput. Aided Chem. Eng.*, 10.

Wieringa, J. A., Dieren, F. van, Janssen, J. J. and Agterof, W. G. M. (1996). Droplet breakup mechanics during emulsification in colloid mills at high dispersed volume fractions. *Trans. Inst. Chem. Eng.*, 74-A: 554-562.