Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
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Integrating batch operations involving liquid-solid mixtures into continuous process flows

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ABSTRACT

This work focuses on modeling batch processes with phase retention, where a portion of the solid or liquid phase is retained after each cycle. While existing simulators primarily model simple batch cycles, this research aims to incorporate batch processes with re-use into flowsheet simulations. Batch processes with phase retention, such as those found in wastewater treatment, biomass hydrolysis and extraction, offer significant advantages, including resource savings and improved process flexibility. These processes introduce a new degree of freedom: the retained phase fraction. The re-use introduces dynamic behavior, as reaction products accumulate in the retained phase over multiple cycles. This necessitates an extended time horizon for mass balance calculations to capture the periodic steady-state. Here a general algorithm is proposed to simulate the periodic behavior of batch processes with re-use for any given kinetics which will enable the integration of these processes into flowsheet simulations.

Keywords: Batch Process, Algorithm, Process Design, Aspen Plus, Simulation.

INTRODUCTION

While there has been a growth in specialized simulators for batch processes, the prevailing trend is towards a simple cycle modeling. Batch processes can be then integrated into an overall flowsheet, with the output stream properties calculated based on the established reaction conditions (time, temperature, etc.).

Moreover, a wide range of *heterogeneous* batch processes exist within industry. Examples include sequential batch reactors (SBR) in wastewater treatment, solid-liquid extraction processes, adsorption reactors and lignocellulosic biomass hydrolysis. When processing solid-liquid mixtures, phase separation can be exploited. In fact, these processes enable the separate discharge of the liquid and solid phases, providing flexibility to selectively retain either phase or a fraction thereof. SBRs retain microbial flocs while periodically discharging a portion of the treated effluent. In biomass hydrolysis, pentoses and lignin solubilize, leaving cellulose as the remaining solid phase. In this case, since cellulose is the fraction of interest, the solid can be separated and most of the liquid phase retained for processing a new batch of biomass, thus saving reagents, water, and energy [1].

APPROACH

In a heterogeneous batch process, a degree of freedom typically emerges that often becomes a decision variable in the design of these processes: the solid-to-liquid ratio ($r\_{S/L}$), which is a critical parameter that influences factors such as reaction rate, heat transfer and cost. Figure 1 illustrates the re-use process, alternatively called Partially Conserved Batch (PCB), in which the solid phase is the desired product. Partial phase retention adds new degrees of freedom to the process design: the retained fractions $f_S = m\_r/m$ for solid and $f_L = V\_r/V$ for liquid phase in which m_r and V_r are the solid and liquid retained mass and volume respectively, while m is the initial input solid mass and V is the initial input liquid volume. The reaction proceeds for a time t_reac.

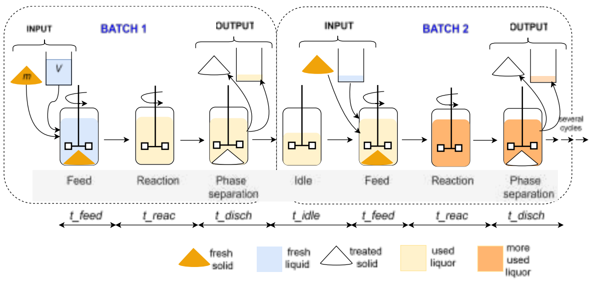

Figure 1: Schematic representation of a PCB.

Subsequently, the treated (wet) solid is removed, and a fresh batch of raw material is introduced along with a make-up liquid to restore the initial liquid volume *V*. In a traditional batch process, the time horizon for analysis corresponds to the reaction, loading and unloading time, and eventually an idle time. For re-use processes, the mass balance will cause reaction products to accumulate in the retained phase from batch to the next. To take this into account, the time horizon for mass balances needs to be extended to include as many cycles as necessary. Eventually, a periodic operating condition will be reached.

An analytical solution for this periodic state can sometimes be found, as demonstrated in [1] for linear reactions. Alternatively, the system of equations can be iterated until two successive cycles converge to within an epsilon. However, the existence of a periodic solution requires a detailed analysis of the relationship between the intrinsic properties of the original system and the batch-with-reuse scheme, using the hybrid impulsive differential equations framework [2]. The primary objective of this work is to incorporate the batch-with-reuse model into flowsheets, like traditional batches, by identifying the periodic state under the given process conditions.

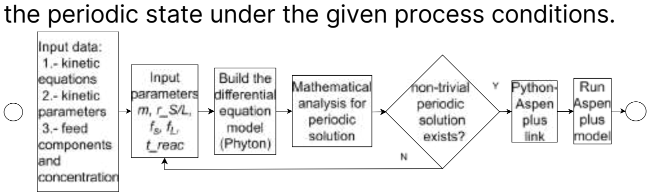

Figure 2: Algorithm for inclusion PCB in Aspen plus flowsheets.

A general algorithm to simulate the periodic condition suitable for any kinetics is proposed (Figure 2). A custom module (**CM**) was created in ASPEN Plus. The connection between Python and Aspen Plus was established using the win32com.client library, which enables communication with Windows applications through COM (Component Object Model). This approach allows the automation of data extraction, input modifications, and simulation execution. The Python script calls the solid input flow from ASPEN Plus and calculates the necessary solvent input. Then, the differential equations are numerically solved for each component, determining the cycles needed for periodicity, such that the maximum concentration difference between successive cycles is below an epsilon. The final periodic concentrations are obtained, and another Python script returns the solid and liquid stream conditions to ASPEN Plus **CM**. Buffer tanks were added upstream and downstream of the PCB reactor within the **CM** to ensure continuous feed and provide a continuous downstream output.

The methodology was tested in the acid hydrolysis of sugar cane bagasse, using the Eqs. (1) and (2) and 1st order kinetic parameters described in [3]. An ε=1E−2 g/L was set. *Gn*, *G*, and *Gd* represent glucan, glucose and glucose decomposition products, respectively; similarly, *Xn*, *X*, and *Xd* represent xylan, xylose and xylose decomposition products.

$$Gn \xrightarrow{k_1} G \xrightarrow{k_2} Gd \qquad (1)$$

$$Xn \xrightarrow{k_3} X \xrightarrow{k_4} Xd \qquad (2)$$

To illustrate, three cases were run, varying only f_L values of 0, 0.5, and 0.9, while keeping a solid mass flow rate of 10 kg/h, *t_reac* = 100 min, *r_S/L* = 10, and f_S = 0 constant. This ODE system is confirmed to exhibit non-trivial periodic conditions across all cases.

RESULTS

Table 1: Simulation results. Final conc. refers to liquid phase

Case study		I	II	III
	f_L	0	0.5	0.9
Final conc. (g/L)	C_G	3.2	6.4	31.9
	C_X	19.5	21.1	22.6
	C_Gd	0.0	0.0	0.0
	C_Xd	0.0	17.9	172
Solvent consumption (kg/h)		100	54	11
Number of cycles to periodicity		1	12	73

Table 1 summarizes the numerical simulation results. Case I corresponds to the traditional batch. The final concentration of the species in the liquid phase refers to the final concentrations of the periodic cycle. The solvent consumption decreases, and the concentration of components increase with f_L. A similar procedure can be applied to any ODE system, after first studying if a periodic condition exists. The **CM** allows for the manipulation of operational parameters, enabling the identification of optimal system operation. Subsequent work will explore the optimization of a comprehensive flowsheet integrating this tool.

REFERENCES

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