A Real Time Simulator of a Supercritical Fluid Extraction (SFE) System

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1. Introduction

Simulators are important aids in the design and development of process applications and also serve as valuable training tools for operators. Simulators are all the more valuable for supercritical fluid extraction (SFE) processes due to the inherent non-linear character of supercritical fluid behaviour. For example, in a SFE process, increasing the heat energy input causes a temperature increase which will also impact pressure. Changes in temperature and pressure then result in a change in the supercritical fluid's density in a manner that is not easy to judge. Changes in temperature, pressure and density then cascade to impacts on component solubility, fluid behaviour, and mass transfer dynamics. All combined, it is difficult to anticipate the overall response of the system to a change in a single input in the absence of a simulator. This difficulty is even more important during the development of new supercritical fluid applications.

In this work, a customized Real Time (RT) simulator of a supercritical fluid extraction process is presented. The simulator is based on first principle mathematical equations, specifically mass and energy balances, fluid mechanics, mass transfer and thermodynamic equations.

The simulator presented is for a SFE process consisting of the following unit operations: an extractor, a separator, pumps, heat exchangers, and throttling valves (referred to as metering valves or MV). The graphical user interface (GUI) of the simulator has been designed and programmed in a flexible manner to allow the user to change different parameters associated with the stated unit operations before and during the simulation. This permits the user to explore the impact of the applied change in real time on process variables such as pressure, temperature, and extract concentration. Building on previous work[1,2], the work presented herein will use the developed simulator to provide an example of system response to a parameter change of a select unit operation. The example will illustrate the simulator's value in predicting responses that are not immediately obvious and highlight how the simulator can be used for development and training purposes.

2. Materials and Methods

The hydrodynamic and mass transfer models which the simulator is based on are detailed in previous work[1,2]. Briefly, the hydrodynamic model is a combination of ordinary differential equations and algebraic equations requiring numerical integration. The mass transfer models are based on mass transfer equations and Chrastil's model for solubility[3]. The Span and Wagner Fundamental Equation of State[4] is used to calculate carbon dioxide's properties.

The developed equations were numerically solved using Simulink® coupled with a program written in C to solve the Fundamental Equation of State relationships.

A customized GUI supports the simulator within the Matlab® framework (Figure 1). The simulator and GUI were programmed and designed to demonstrate main unit operations of a continuous SFE process. After the development of the simulator and its GUI, a series of simulations were conducted to explore the impact of different operating conditions in real time on various process variables, specifically pressure, temperature, and extract (oil) concentration.

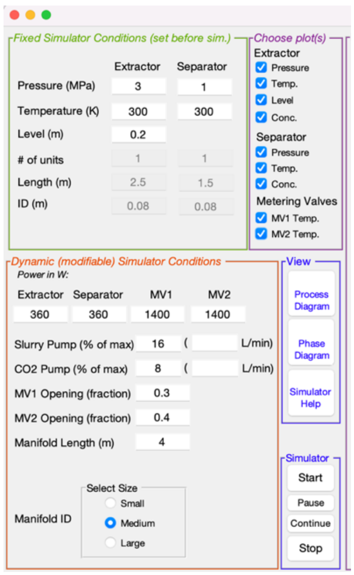

Figure 1. Simulator GUI

3. Results and Discussion

Figure 2 illustrates the system startup and dynamic response (the first 1000 s) to a generic set of initial conditions associated with the continuous SFE process. The results show an increase in extractor pressure that is far from a simple asymptotic approach to steady state. The extractor pressure overshoot is not intuitively obvious and is linked to the complex interdependence of extractor pressure on extractor temperature and on separator pressure and temperature.

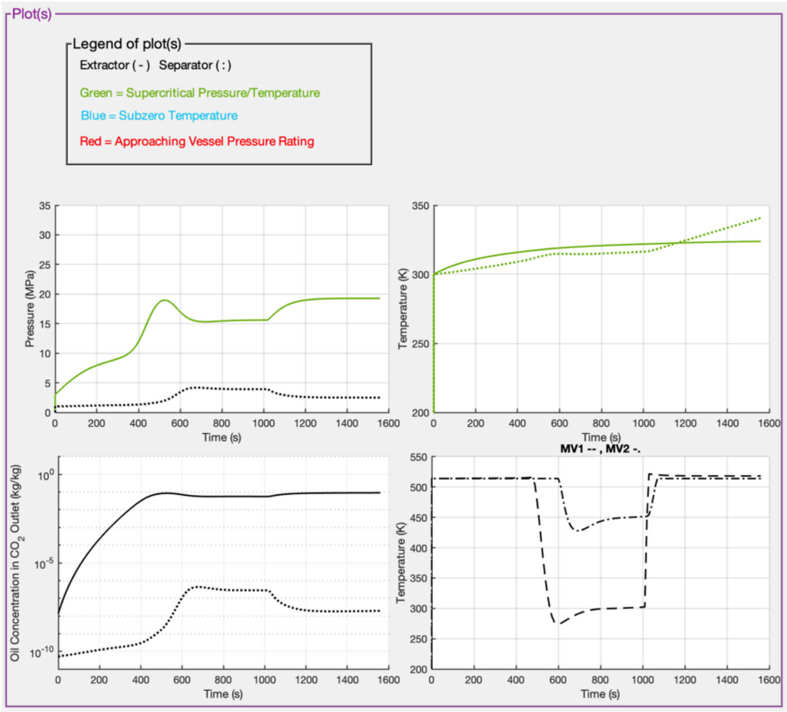

Figure 2. RT simulation results for startup and change in heat input to MV1

At approximately 1000 s, the heat input to the metering valve between the extractor and separator was increased (MV1; from 1400 to 2800 W). This leads to an increased temperature within MV1 and the separator as one would expect. But surprisingly, it also leads to an extractor pressure increase. The increased MV1 heating changes the CO_2 properties flowing through the valve, leading to a flow reduction through the valve. The lower flow through the valve increases the extractor pressure while decreasing the separator pressure. As seen in Figure 2, these changes in extractor pressure and separator pressure, result in an increase and decrease of oil concentration in extractor outlet and separator outlet, respectively.

4. Conclusions

In this work, the value of a real time simulator of a SFE process (or SFE processes in general) is demonstrated. The presented simulator and its GUI are applied to showcase a scenario in which system responses are difficult to anticipate due to the inherent non-linear behaviour of SFE processes. A customized and flexible SFE process simulator serves as an important tool for the development of SFE processes for a variety of applications and as a valuable training tool for operators.

References

1. M. Roodpeyma, PhD Thesis, Dept. of Civil & Env. Eng. University of Alberta, **2017**.
2. C. Street, PhD Thesis, Dept. of Civil & Env. Eng. University of Alberta, **2021**.
3. J. Chrastil, J. Phys. Chem., **1982**, 86, 3016.
4. R. Span, W. Wagner, J. of Physical Chem. Ref. Data **1996**, 25, 1509.