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BatchReactor Application Example

Simulation of a Pressure Increase Scenario in a Two-Phase Reactor

Example purpose
This example presents a simple case of pressure increase of a tank, followed by a depressurization after the rupture disc breaks out. The characteristics of the flow at the vent and the evolution of the tank load are followed over time.

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Corresponding BatchReactor file	*BATCHREA_EX_EN-Pressure-increase.pbpr*

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1. INTRODUCTION

This example deals with the study of a scenario of pressure increase of a capacity. During the first step, the tank (being closed) is subjected to a thermal flow, the pressure increases up to the breaking pressure defined for the rupture disc. During the second step, the tank is depressurized with a vent flowrate assumed to be constant. Finally, the reactor evolves at atmospheric pressure.

In this simple case, no reaction nor heating device is taken into account.

2. COMPONENTS

The components that take part into the simulation appear in the table below:

Name	Formula	CAS Number[1]
Water	H_2O	7732-18-5
Methanol	CH_4O_2	67-56-1
Nitrogen	N_2	7727-37-9

The compounds are taken from the Simulis Thermodynamics standard database, thermodynamics calculation engine used in BatchReactor. The thermophysical properties stored in this database are the DIPPR recommended values [ROW23].

3. THERMODYNAMIC MODEL

The NRTL [REN68] thermodynamic model is used to model the phase equilibria. Binary interaction parameters for the water-methanol binary are taken from the Simulis Thermodynamics database. No binary interaction parameter have been defined for the water-nitrogen and methanol-nitrogen binaries.

[1] *CAS Registry Numbers® are the intellectual property of the American Chemical Society and are used by Fives ProSim SAS with the express permission of ACS. CAS Registry Numbers® have not been verified by ACS and may be inaccurate.*

4. SIMULATION

4.1. Process description

4.1.1. Reactor

The reactor used in this example is a closed two-phase vapor-liquid reactor. Its volume is 200 l. The reactor head space is initially inerted with nitrogen.

The initial conditions appear in the table below:

Initial conditions	
Temperature	25°C
Pressure	1 atm
Initial load	
Total load	50 l
Water	50% mol.
Methanol	50% mol.

The alarms are as follows:

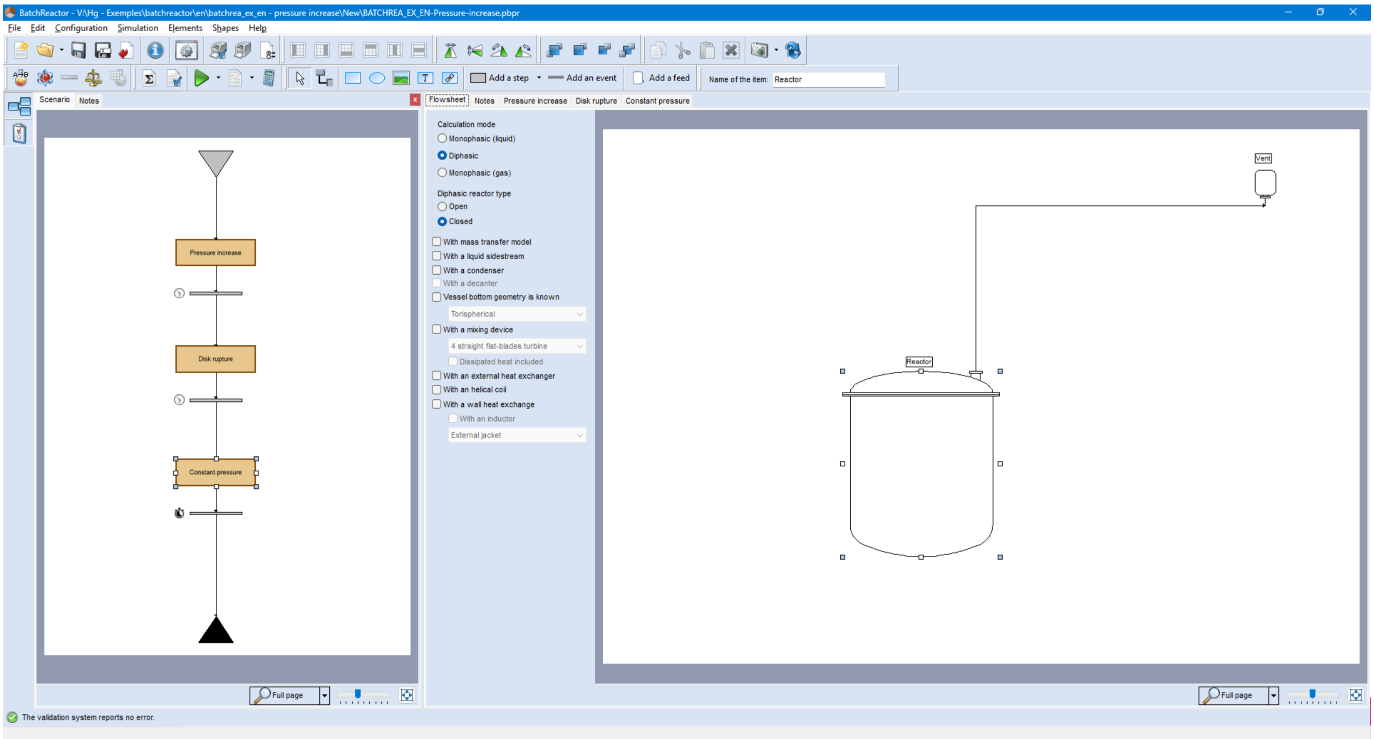
	Volume	Temperature
Minimum	1 l	0°C
Maximum	190 l	200°C

4.1.2. Operating mode

The operating mode is made up with three steps. During the first step, the pressure increases inside the tank up to the pressure defined for the rupture disc. The second step models the depressurization resulting from the breaking of the disc. During the third step, the reactor evolves at atmospheric pressure.

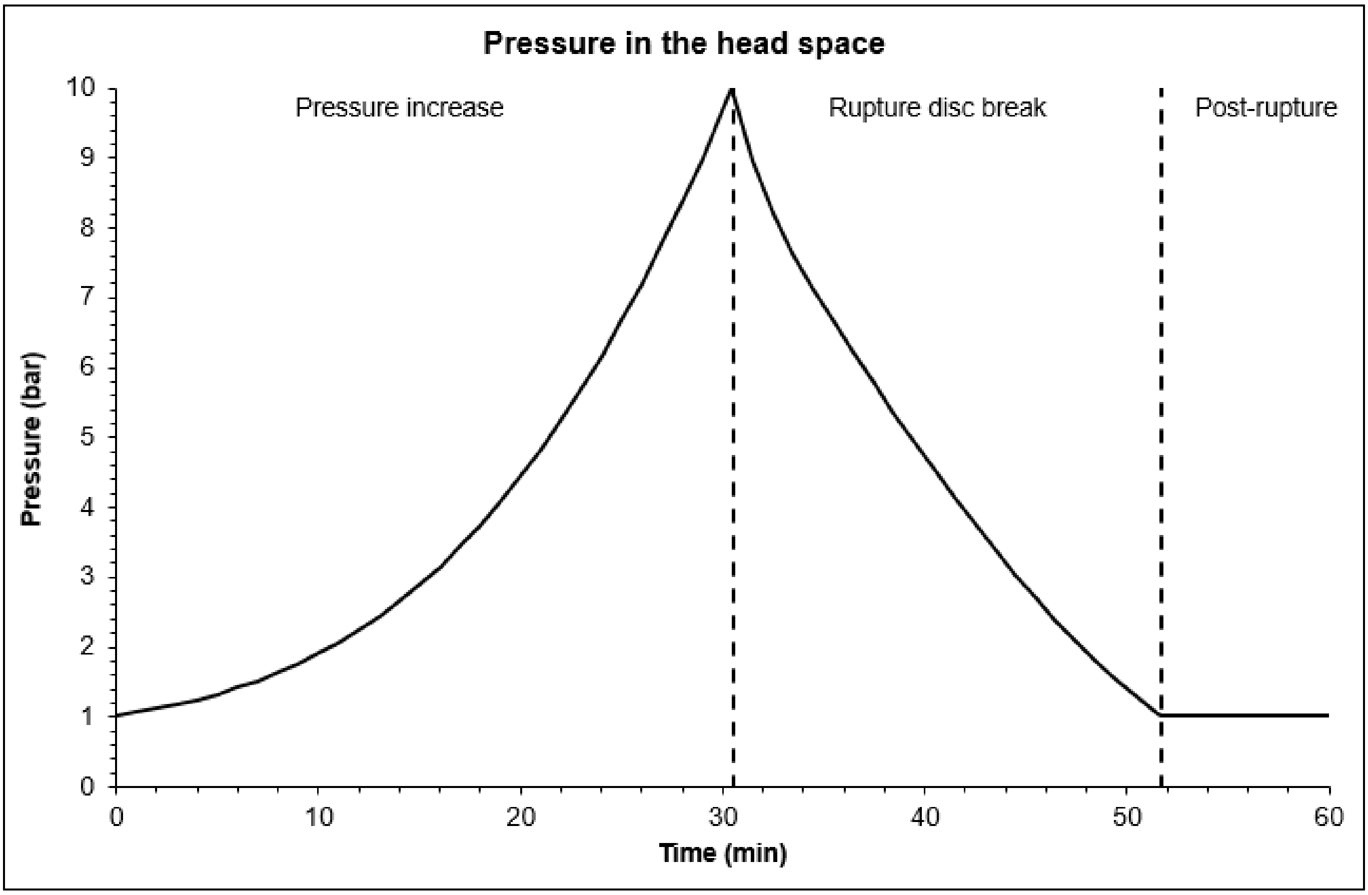
Parameter	Step 1	Step 2	Step 3
Type	Specified heat duty		
Heat quantity	10 kW		
Pressure specification	Constant vapor flowrate		Constant pressure
Vapor production	0 kg/h	50 kg/h	-
Reactor pressure	-		1 atm
Stop event	Pressure in the reactor = 10 bar	Pressure in the reactor = 1 atm	Duration of simulation = 1 h

The scenario is presented on the left of the following screenshot and the flowsheet on the right part.

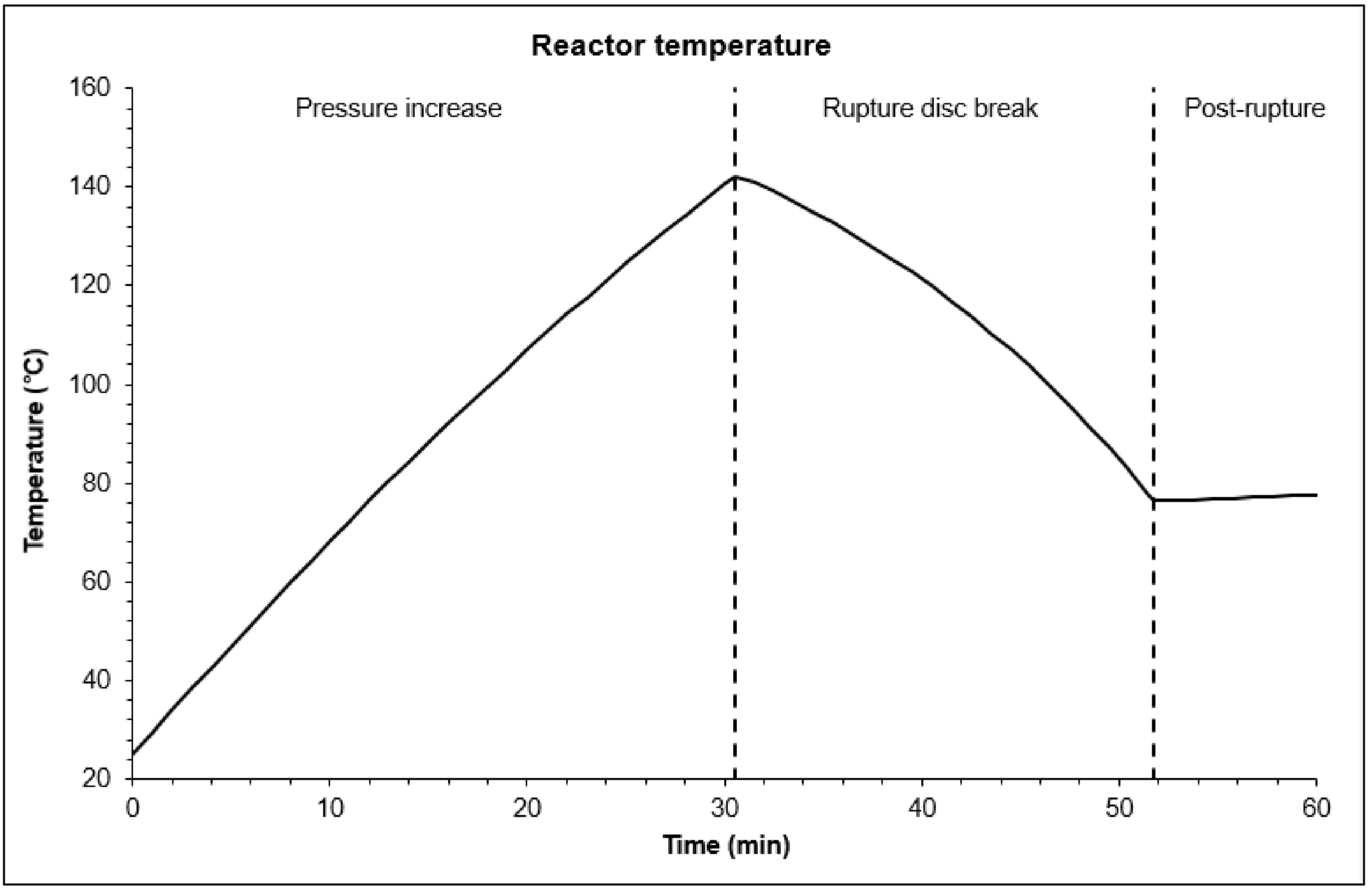


4.2. Results

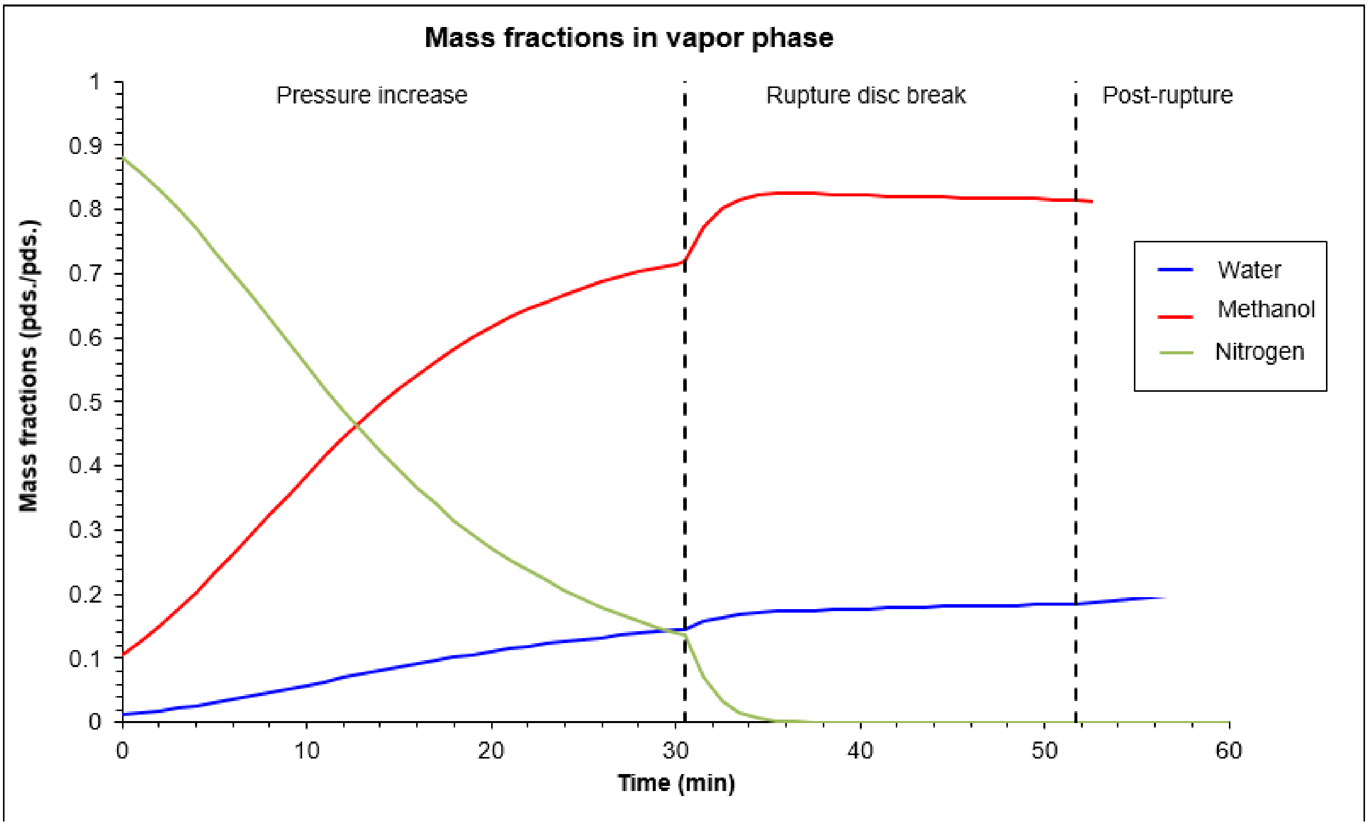
The following graph shows the pressure evolution in the reactor head space. As long as the pressure is lower than the breaking pressure of the rupture disc (with the vent closed and the heating process running), the pressure inside the reactor increases as a result of the vaporization of the load. The breaking pressure of the rupture disc (10 bar) is reached in just over 30 minutes.



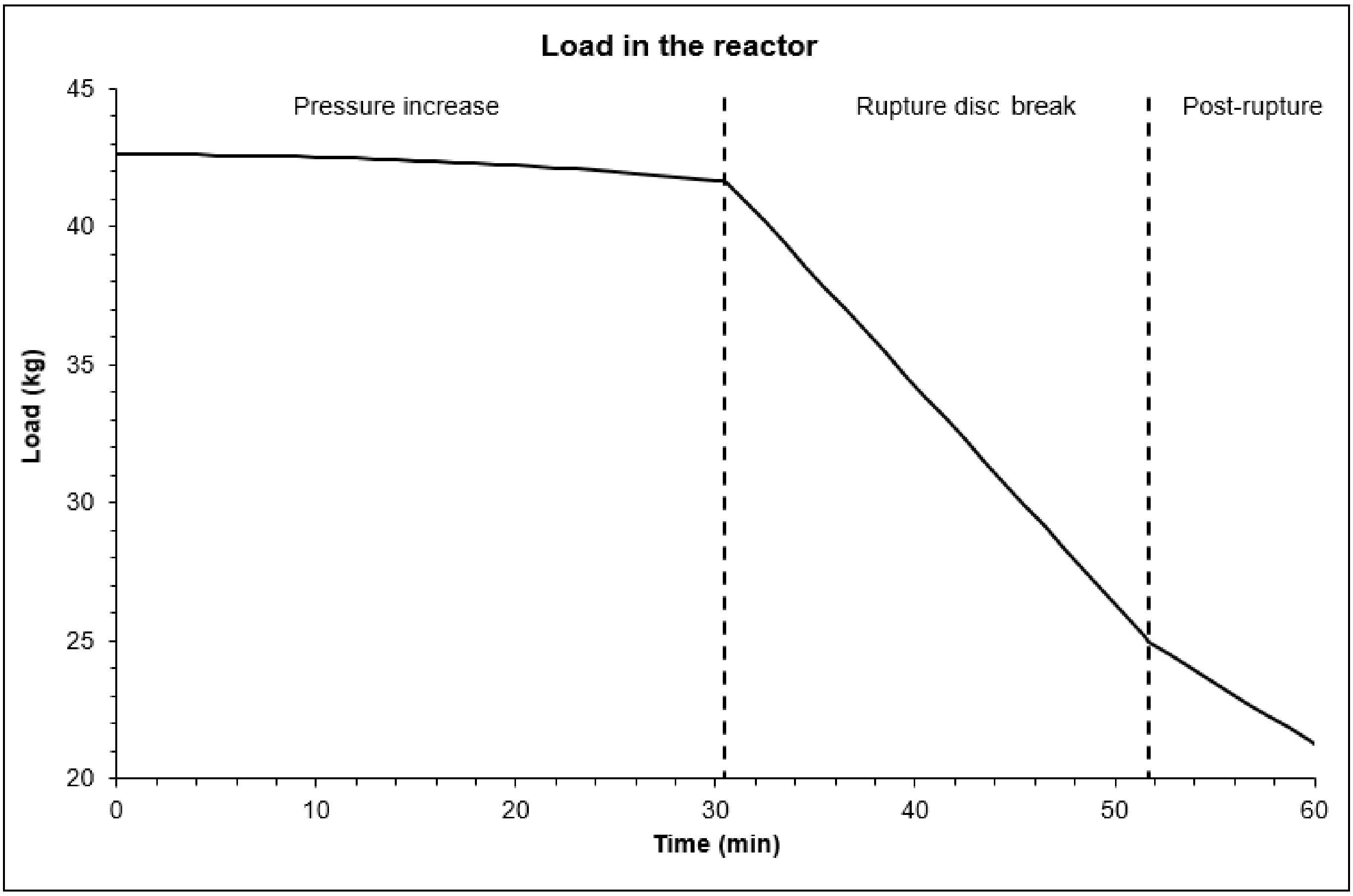
The following graph shows the evolution of the temperature in the reactor. It increases during the pressure increase phase as a result of the heating of the tank. The depressurization that occurs after the rupture disc break leads to a temperature decrease due to the evaporation of part of the load. In the last phase, the system has reached the equilibrium and the temperature increases again due to the heating of the reactor.



The following graph shows the evolution of the composition of the gas phase in the reactor. The composition of the gas that leaves the reactor after the rupture disc break is found in the **Rupture disc break** part of the graph below. It is made up of 80% of methanol (mass) and 20% of water (mass).



The following graph shows the evolution of the load in the reactor. It shows that almost 40% of the initial mass load is vented away when the rupture disc breaks out.



5. References

[REN68] RENON H., J.M. PRAUSNITZ, “Local Compositions in Thermodynamic Excess Functions for Liquid Mixtures”, AIChE J., 14(3), 135-144 (1968)

[ROW23] ROWLEY R.L., WILDING W.V., OSCARSON J.L., GILES N.F., “DIPPR® Data Compilation of Pure Chemical Properties”, Design Institute for Physical Properties, AIChE (2023)