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CFD simulation of shortstopping runaway reactions in vessels agitated with impellers and jets

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Abstract

Runaway reactions are continuing to be a problem in the chemical industry. A recent study showed that 26% of our major chemical plant accidents are due to runaways. The consequences of runaway reactions are usually mitigated with (a) reliefs and containment systems or (b) shortstopping (reaction inhibition). This study covers the concept of shortstopping.

One of the major reasons for runaways is power failure. In the advent of a power failure, mixing an inhibiting agent with the reactor contents is challenging. However, jets or impellers driven by a small generator can be used for mixing. This study compares shortstopping results in vessels agitated with jets and impellers using computational fluid dynamics (CFD). A commercial CFD code, Fluent is used.

For shortstopping systems relying on jet mixing, angle and diameter of jet nozzle and jet velocity are the key design/operating parameters. For the systems with impellers, type, size and RPM of impeller are the key parameters. In this work, mixing with a jet mixer is first investigated for three nozzle diameters and two angles of injection. The best jet mixer configuration on the basis of mixing time is used for shortstopping studies. The simulated shortstopping results with the jet mixer are then compared with those obtained with impeller (Rushton and pitched blade turbine) stirred vessels. Our results identify the conditions for effective shortstopping; i.e., agitation requirements, locations for adding the inhibitor, and the quantity of inhibitor.

The distribution of excess inhibitor is shown to be an important and essential design criterion for effective shortstopping when using impeller stirred vessels. The comparative study with a single jet shows that jet mixer is ineffective when used for shortstopping. Efforts such as adding excess inhibitor and inhibition with higher reaction rates at the same power, proved to be ineffective when using jet mixer compared to the results with impellers.

Keywords: Jet mixer; Impeller stirred vessels; Runaway reaction; Shortstopping; CFD

1. Introduction

Runaway reactions are continuing to be a problem in the chemical industry. A recent study showed that 26% of major chemical plant accidents are due to runaways (Balasubramanian & Louvar, 2002). One of the major reasons for runaways is power failure. The loss of agitation triggers the loss of temperature control, which leads to the heating of the reactor contents and runaways. Runaway reactions are usually mitigated with (a) reliefs, (b) reliefs and containment, or (c) shortstopping. The most commonly used method is reliefs and containment. Shortstopping is used only occasionally because the technology is not fully developed; there are only a few references (Hoffman, 1996; Kammel, Schluter, Stefiff, & Weinspach, 1996; Mewes & Renz, 1991; Schimetzek, Steiff, & Weinspach, 1995) available that discuss shortstopping and there are no guidelines or standards.

Runaway reactions can be inhibited in two ways, namely by the addition of cold diluents and by the addition of an inhibitor (chemical reaction stopper). In the advent of a

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Nomenclature

Cw_i	mass fraction of species i, kg(i)/kg(total)
c_p	specific heat, J/kg(total) K
CMF	completely mixed flow
CFD	computational fluid dynamics
D_i	impeller diameter, m
D_j	jet nozzle diameter, m
D_o	outlet diameter, m
d_s	shaft diameter, m
E	activation energy, J/kg mol
F	mixing time factor
g	acceleration due to gravity, m/s^2
H	height of liquid from the bottom of the reactor, m
ΔH	heat of reaction, J/kg(monomer)
k_0	pre-exponential factor for the first reaction, kg(total)/(kg(cat) h)
k_1	pre-exponential factor for the second reaction, kg(total)/(kg(inh) h)
N	impeller rotational speed, rps
N_p	power number
P	power consumption, W
PBT	pitched blade turbine
Δp	static pressure difference between inlet and outlet, Pa
Q	mass flow rate through the jet, kg/s
Re	Reynolds number
RT	Rushton turbine
T	vessel diameter, m
Temp	temperature, K
t	time, h
t_{99}	mixing time (99% homogeneity), s
t_{95}	mixing time (95% homogeneity), s
t_r	runaway time, s
V_j	inlet jet velocity, m/s
V_o	outlet velocity, m/s
ΔZ	difference in the height between inlet and outlet, m

Greek letters

ρ	density, kg/m^3
μ	viscosity, Pa s
α	angle of injection

power failure, adding an inhibiting agent and mixing it with the reactor contents is challenging. However, jets or impellers (Rushton or pitched blade turbine) driven by a small generator can be used.

It has been reported that (a) jet mixing can be used to mix the inhibitor into a monomer storage tank to stop runaway reactions (Hoffman, 1996; Kammel et al., 1996; Mewes & Renz, 1991) and (b) jets can be used to facilitate cooling systems when agitation fails (Schimetzek et al., 1995). Even though jet mixer is reported to be a viable mixing device in the shortstopping process, none of the previous references predict the effectiveness of jets.

The effectiveness of shortstopping using jet mixers (and other means of agitation) cannot be easily determined with laboratory and pilot plant scale experiments due to the hazards associated with runaway reactions. In this work, we use computational fluid dynamics (CFD)-based models to study the concept of the shortstopping process and to develop design criteria. The effectiveness of jet mixed vessels in shortstopping is compared with vessels stirred with impellers.

From a design standpoint, jet mixing is one of the simplest methods to achieve mixing. In jet mixing, a part of the liquid in the tank is drawn through a pump and returned as a high-velocity jet through a nozzle into the tank (Patwardhan, 2002). This jet mixes the fluid by entraining some of the surrounding liquid and creating a circulation pattern within the vessel. Fossett and Prosser (1949) were the first to investigate jet mixing. Fox and Gex (1956) then studied jet mixing in both laminar and turbulent regimes using axial vertical jets. Their results indicate that mixing time is dependent on the jet Reynolds number; the dependence being strong in the laminar region but weak in the turbulent region. Lane and Rice (1982a, b) extended the investigation to inclined side entry jets. They developed a mixing time formula that is used to predict 95% homogeneity. An improved correlation giving a better fit of mixing time data for turbulent jet mixed vessels was proposed by Grenville and Tilton (1996). Brooker (1993) was the first to study the performance of a jet mixer using CFD, and Ranade (1996) investigated the flow patterns in jet mixed tanks using CFD simulations.

Jayanti (2001) used a general-purpose CFD code, CFX, to investigate the hydrodynamics of jet mixing in cylindrical vessels. He found the key factor in reducing the mixing time is by minimizing or eliminating dead zones in the reactor. Patwardhan (2002) presented a CFD model, which predicted the mixing time with experimental validation. Patwardhan and Gaikwad (2003) extended the investigation and studied the effect of the diameter of the jet on the mixing time. They also compared the efficiency of jet mixers over conventional impeller stirred vessels on the basis of equal power consumption. They reported that one could achieve better mixing with jets than with impellers (with equal power consumption) by increasing the jet diameter. Zughbi and Rakib (2002) presented a CFD model of jet mixing and validated their numerical model against the experimental results from Lane and Rice (1982b). Zughbi and Rakib (2004) extended their investigation to study the influence of jet angles on mixing times. They reported that a 30° inclination gives better mixing than 45° inclination.