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CFD simulations for safety of chemical reactors and storage tanks

Leszek Rudniak[a] , Aleksandra Milewska[b] and Eugenisz Molga[c]

[a]*Warsaw University of Technology, Chemical and Process Engineering Department, ul. Warynskiego 1, 00-645 Warszawa, Poland, rudniak@ichip.pw.edu.pl*
[b]*Institute of Power Engineering, Department of Thermal Processes, ul. Agustówka 36, 00-891 Warszawa, Poland, aleksandra.milewska@ien.com.pl*
[c]*Warsaw University of Technology, Chemical and Process Engineering Department, ul. Warynskiego 1, 00-645 Warszawa, Poland, molga@ichip.pw.edu.pl*

Abstract

Two CFD models have been formulated for the stirred tank reactor and the storage tank, respectively. Spatial and time profiles of the liquid velocity, temperature and concentration inside the reactor and storage tank have been determined for different thermal runaway scenarios. The obtained results indicate that the CFD models can be very useful to elaborate an efficient and robust method for on-line early runaway detection.

Keywords: CFD modeling, safety aspects, heat and mass transfer, exothermic reactions

1. Introduction

In chemical reactors, in which strongly exothermic reactions are carried out as well as in tanks used to store thermally sensitive chemical compounds a loss of temperature control (thermal runaway) can occur. In chemical reactors it can be provoked, when for some reasons the rate of heat generation due to the reaction progress exceeds the rate of heat removal by cooling. In such a case an auto-acceleration effect can be observed – i.e. this local temperature increase accelerates the reaction rate, then it in turn increases the heat generation rate and in consequence also the temperature of the reactor content. In storage tanks a local temperature increase, can trigger off a thermal decomposition reactions, which usually are very exothermic and can lead to further temperature increase and even explosion. In chemical industry, despite significant improvements in safety analysis, still a lot of thermal runaway events is noticed [1,2].

The model based safety analysis is the most efficient and robust method to prevent thermal runaway, because it helps to find safe or even inherently operating conditions. In particular, CFD (Computational Fluid Dynamics) models can be very useful for this purpose. These models allow to obtain a solution of conservative equations derived for mass, momentum, energy and species in any reacting system. CFD simulations can supply a relevant information on a dynamic behavior of the modeled system – particularly the time and spatial profiles of fluid velocity, temperature and concentrations can be determined within the modeled vessel (reactor or storage tank). So, different runaway scenarios can be simulated for the vessel of any geometry and configuration as well as at different mixing conditions. These "computational experiments" carried out with use of CFD models can be very useful, particularly for industrial processes, where safety experiments carried out in real installations are very expensive and dangerous. Several contributions devoted CFD applications to study runaway reactions can be found in the literature of subject [3-8].

In this paper an ability of CFD models to asses safety of stirred tank chemical reactors and storage tanks is presented and discussed.

2. CFD models formulation for chemical reactors and storage tanks

For the purpose of these studies, two types of CFD models has been elaborated – i.e. for batch stirred tank reactor as well as for storage tank of chemical compounds. Each CFD model formulated for the systems listed above, consisted of a set of conservation equations for mass, momentum, energy and species. The general balance equation over the element volume of reactor or storage tank can be written for each system variable ϕ as follows (in Cartesian system of coordinates):

$$\underbrace{\frac{\partial \phi}{\partial t}}_{\text{Accumulation of } \varphi} + \underbrace{u_i \frac{\partial \phi}{\partial x_i}}_{\substack{\text{Change rate of } \varphi \\ \text{due to convection}}} = \underbrace{\frac{\partial}{\partial x_i}\left(\Gamma_i \frac{\partial \phi}{\partial x_i}\right)}_{\substack{\text{Change rate of } \varphi \\ \text{due to diffusion}}} + \underbrace{S_\phi}_{\substack{\text{Change rate of } \varphi \\ \text{due to sources}}} \tag{1}$$

A strongly exothermic, homogeneous reaction carried out in a single and incompressible liquid phase has been considered, to define the appropriate terms for heat and mass source, as they appear in the balance equations – see Eq. (1). In the stirred tank reactor the esterification reaction between the propionic anhydrite and the iso-propanol has been considered, while for the storage tank the first order thermal decomposition reaction of liquid filling the tank has been chosen.
In stirred tank reactors the motion of fluid is enforced by a rotating impeller, so the specific methods, such as the moving reference frame method (MRF) and the sliding mesh one (SM), have been applied to calculate flow filed – for details see [8]. In storage tanks a free convection of mass and heat have been taken into account. Additionally, during formulation of CFD models the vessel geometry and mesh generation as well as the appropriate turbulence model have to be defined. In our studies the k-ε turbulence model has been utilized.

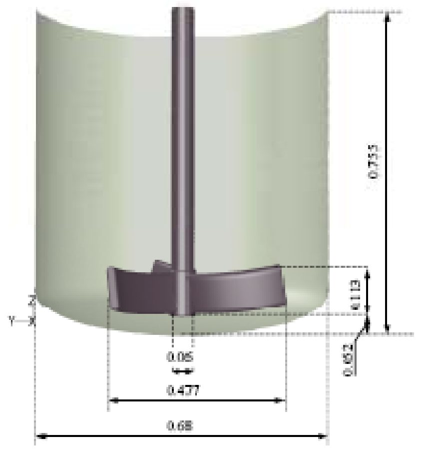


Fig.1. The main dimensions of the modeled pilot plant stirred tank reactor (values in meters)

In a 3D CFD model formulated for the stirred tank reactor, the geometry and mesh have been implemented using the MIXIM software, improved with GAMBIT and TGrid packages. The main dimensions of this pilot plant reactor of the nominal volume of 340 dm^3 are shown in Fig. 1 [8]. In a case of the storage tank due to a spherical symmetry, a 2D CFD model has been elaborated, where the tank geometry and mesh have been defined with the GAMBIT package. A spherical storage tank of diameter of D = 5 m, containing the compound, which properties are similar to the petrochemical oil has been chosen as a case study.
For both types of elaborated CFD models the appropriate boundary conditions and simulation parameters, such as type of solver, near wall treatment, discretization, under-relaxation factors, convergence criteria and iteration parameters have been applied [9]. These models have been solved with use of the FLUENT software package [9].

3. Results and discussion

A main aim of the performed simulations was to predict a dynamic thermal behavior of the typical industrial stirred tank reactor as well as the large-scale storage tank, in a case of unexpected circumstances, which can lead to thermal runaway. The elaborated CFD models make possible a versatile safety analysis of both considered systems as well as carry out investigations of different runaway scenarios.
In a case of the considered stirred tank reactor, the CFD model makes possible a determination of safety operating conditions – i.e. a prediction for any run (at any initial and operating conditions) whether the process can be executed safely or even inherently safely. For such a run, spatial and time profiles of the velocity, temperature and concentration have been obtained as a result of the performed CFD simulations. Typical temperature profile inside the reactor at the chosen time moment is shown in Fig. 2.

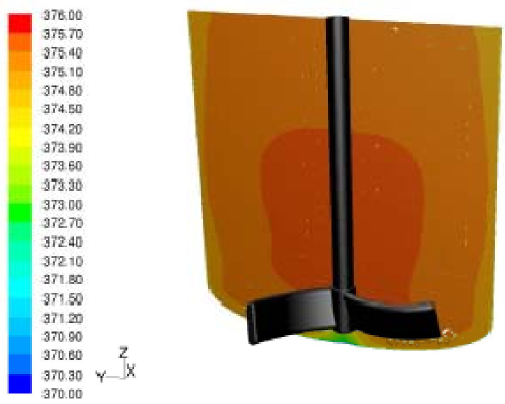


Fig. 2. Temperature profile inside the stirred tank reactor at the specific time moment. Results obtained for a normal reactor operation with use of the CFD model for esterification reaction carried out at the constant reactor jacket temperature equal to T_J = 348 K.

In Fig. 2 a quite uniform temperature distribution inside the reactor can be observed, despite a fact that the nominal volume of considered reactor is rather large. In the considered case a mixing intensity of the reactor content is good enough, so the maximal difference of temperature measured at different locations is as small as approx.

0.9 K. In such a case the localization of single temperature sensor inside the reactor is not significant for on-line detection of thermal runaway and early warning.

To describe the entire process, from the spatial temperature distribution obtained with the CFD model also a volume-averaged temperature inside the reactor can be estimated as a function of time.

However, the elaborated CFD reactor model has a great significance particularly for predicting the reactor behavior in a case of the simulated fault of stirring system– e.g. stirrer damage and stopping. In this situation a more pronounced non-uniformity of temperature distribution is expected, so localization of the temperature sensor is crucial for early enough runaway detection. For this case, typical temperature profile inside the reactor at the chosen time moment is shown in Fig. 3. As can be observed in Fig. 3, due to no-mixing of the reactor content, a non-uniform temperature distribution inside the reactor is more pronounced than during normal operation and the maximal difference of temperature measured at different locations is equal approx. to 3 K.

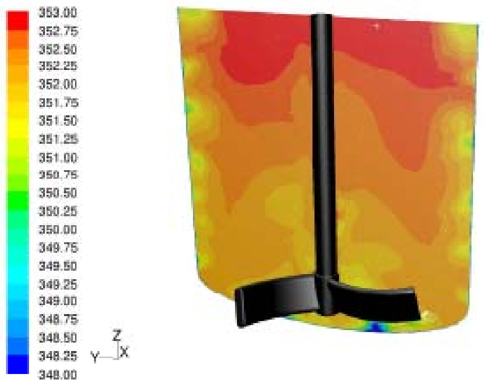
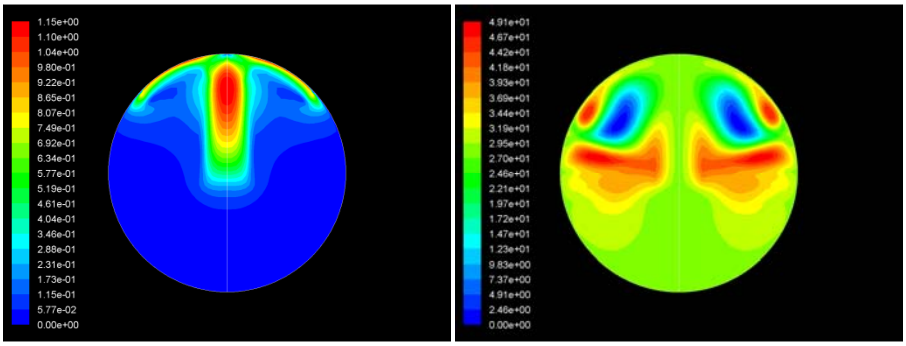


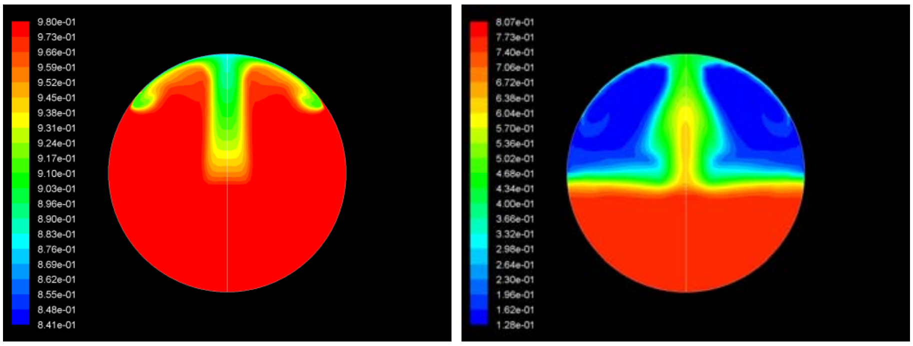
Fig. 3. Temperature profile inside the stirred tank reactor at the specific time moments. Results obtained with CFD model for esterification reaction carried out at the constant reactor jacket temperature equal to T_J = 348 K and for a simulated stirrer damage (results taken for the time moment t = 300 s after stirrer stopping).

The problem of non-uniform temperature and concentration distributions inside the vessel is mostly pronounced in storage tanks, where the heat and mass transfer during thermal runaway are controlled by natural convection, only.

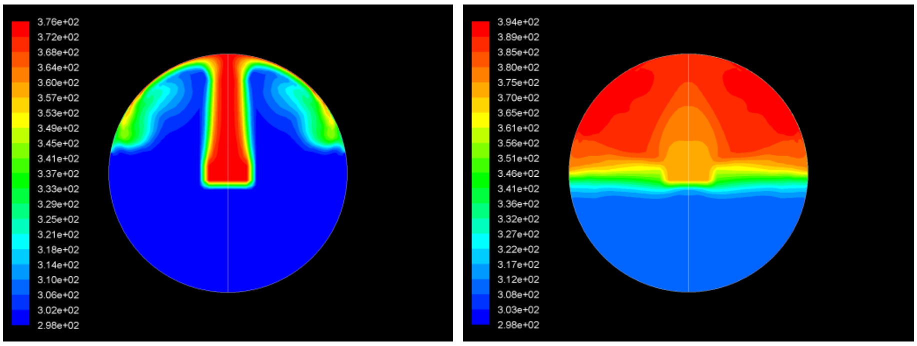
In diagrams shown in Figs. 4a-3c the results obtained with the CFD model elaborated for a storage tank containing thermally non-stable chemical compound, are shown. In this case the thermal runaway is initiated in the center of the tank – e.g. due to a local temperature increase caused by a mistake of the operator or by natural forces. This local temperature increase is propagated within the whole vessel, leading to a global thermal runaway. Distinct “hot-spots” travelling inside the storage tank can be observed in Fig. 4c. The obtained results indicate, that in this case the maximal temperature difference inside the tank vessel is as large as 96 K. These results indicate how important is localization of the temperature sensors and they can help to estimate how many sensors should be installed and where they should be placed to assure an efficient and robust on-line control.



a. velocity profiles in liquid at t = 10 and 100 s, respectively



b. concentrations of the reacting specie at t = 10 and 100 s, respectively



c. temperature profiles at t = 10 and 100 s, respectively

Fig. 4. Velocity, concentration and temperature profiles inside the storage tank at two different time moments. Results obtained with CFD model for thermally non-stable liquid filling the storage tank. Thermal runaway event caused by unexpected temperature increase the tank center.

4. Summary and conclusions

Two CFD models have been formulated for the stirred tank reactor and the storage tank, respectively. With use of the elaborated models a dynamic behavior of the considered systems at different operating conditions has been predicted. Spatial and time profiles of the liquid velocity, temperature and concentration inside the reactor and storage tank have been determined. Different thermal runaway scenarios have been simulated, including those caused by a damage of the reactor stirrer as well as by a triggering off the decomposition reaction in the storage tank. The obtained results indicate that the CFD models can be very useful to estimate the number and localization of temperature sensors, which are able to assure an efficient and robust on-line early detection of approaching thermal runaway.

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References

[1] K.R. Westerterp and E. Molga, Chem.Eng.Res. Des., 84 (2006) 543
[2] F. Stoessel, Thermal safety of Chemical Reactors – Risk Assessment and Process Design, Wiley-VCH Verlag GmbH&Co. KGaA, Weinheim, 2008
[3] U. Kammel, S.Schluter, A. Steiff and P.M. Weinspach, Chem.Eng.Sci., 51 (1996) 2253
[4] H.V. Hristov, K.C. Middle and R. Mann, Chem.Eng.Res. Des., 80 (2002) 872
[5] D. Dakshinamororthy, A.R. Khopkar, J.F. Louvar and V.V. Ranade, J. Loss Prevention Proc. Ind., 17 (2004) 355
[6] L. Rudniak, P.M. Machniewski, A. Milewska, E. Molga, Chem.Eng.Sci., 59 (2004) 5233
[7] A. Milewska, E. Molga, Chem.Eng.Sci., 62 (2007) 4920
[8] A. Milewska, Modelling of batch and semibatch reactors-safety aspects, Ph.. Thesis, 2007 – http:/www.ichip.pw.edu.pl/milewska/thesis_Milewska.pdf
[9] FLUENT 6.1., User guide, 2002.