Applied Thermal Engineering 70 (2014) 451–461

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng

Investigation of flow and heat characteristics and structure identification of FLiNaK in pipe using CFD simulations

C.S. Sona [a], Makrand A. Khanwale [a], Channamallikarjun S. Mathpati [a, *], Ananta Borgohain [b], Naresh K. Maheshwari [b]

[a] Department of Chemical Engineering, Institute of Chemical Technology, Matunga, Mumbai, Maharashtra 400019, India
[b] Chemical Reactor Division, Bhabha Atomic Research Centre, Anushakti Nagar, Mumbai 400085, India

HIGHLIGHTS

- Large Eddy Simulations carried out at different Reynolds numbers.
- Simulations validated using DNS data.
- Local turbulent information extracted using wavelets.
- Heat transfer characteristics calculated using local turbulent information.
- Results match the experimental results with less than 10% variation.

ARTICLE INFO

Article history:
Received 15 January 2014
Accepted 12 May 2014
Available online 24 May 2014

Keywords:
Molten salt
FLiNaK
LES
Heat transfer
Turbulent structures

ABSTRACT

The demand for hydrogen as a transportation fuel is rising day by day. Hydrogen can be produced thermo-chemically or electrolytically at high temperatures. A fluoride salt with eutectic composition of 46.5%LiF–11.5%NaF–42%KF (mol %) commonly known as FLiNaK is a leading candidate for heat transfer fluid. It can be used for transferring heat from high temperature heat source to hydrogen production plant. Computational fluid dynamics (CFD) simulations at three Reynolds numbers were carried out using large eddy simulation (LES) to investigate the flow and heat characteristics of molten FLiNaK in a cylindrical pipe. Simulation results have been validated with the help of mean velocity profile using direct numerical simulation (DNS) data. Transient velocity information was used to identify and characterise turbulent structures which are important for transfer of heat across solid–fluid interface. A wavelet transform based methodology called wavelet transform modulus maxima (WTMM) was used to identify and characterise the singularities. WTMM analysis was also used for flow visualisation, and to calculate heat transfer coefficient using small eddy model. The predicted Nusselt number showed good agreement with the available experimental data.

1. Introduction

Hydrogen, being a clean fuel, is a promising alternative to crude oil as a transportation fuel. Hydrogen can be produced by thermo-chemical [1] or high-temperature electrolysis [2] processes. The sulphur-based cycles, which are currently the baseline thermo-chemical cycles, require heat source at a temperature of at least 850 °C. High temperature electrolysis involves the splitting of water into hydrogen and oxygen at temperatures in the range 750 to 900 °C. The primary advantage of high-temperature electrolysis over conventional electrolysis, is that considerably higher hydrogen conversion efficiencies can be achieved at the higher temperatures [2]. Heat transfer fluids that can withstand high temperatures are required to transfer the heat from high temperature heat source to hydrogen production plant. A fluoride salt with eutectic composition of 46.5% LiF–11.5% NaF–42% KF (mol%) commonly known as FLiNaK, is proposed as the heat transfer coolant due to its superior thermo-physical properties such as high boiling point, low vapour pressure, high thermal conductivity and good stability at high temperature. For a reliable design of heat transfer loop, it is necessary to characterise the thermal hydraulic performance of FLiNaK.

Experimental investigations of heat transfer characteristics are available in the literature [3–6]. However, due to problems associated with high temperature, only overall heat transfer

* Corresponding author. Tel.: +91 22 33612016; fax: +91 22 33611020.
E-mail address: cs.mathpati@ictmumbai.edu.in (C.S. Mathpati).

http://dx.doi.org/10.1016/j.applthermaleng.2014.05.043
1359-4311/

measurement is possible, and there is a need to understand the fundamental heat transfer process. In order to understand fundamental heat transfer at solid–fluid interface with molten salts, computational fluid dynamics (CFD) is essential. Therefore CFD simulations have been carried out in present study to investigate the turbulent flow characteristics of FLiNaK salt in pipe. Simulations have been performed using two different turbulence models (I) standard $k-\varepsilon$ model and (II) large eddy simulation (LES). Simulation results have been validated with the help of mean velocity profile using Direct Numerical Simulation (DNS) data from the literature. The transient velocity information was used to isolate turbulent structures using wavelet transform modulus maxima (WTMM) methodology. The heat transfer characteristics have been investigated in terms of Nusselt number (Nu) and compared with the experimental data available in the literature.

2. Previous work

In this section, previous literature on (i) experimental and CFD studies on heat transfer characteristics of molten salt FLiNaK (ii) turbulent flow structure identification and characterisation have been reported.

2.1. Experimental and CFD studies on heat transfer characteristics of molten salt FLiNaK

Many studies [3–6] on heat transfer characteristics (heat transfer coefficient (HTC) and Nusselt number, Nu) of FLiNaK have been published (Table 1). Grele and Gedeon [3] performed measurements using FLiNaK flowing through an electrically heated horizontal test section. The test section was fabricated from Inconel-X tubing having an outside diameter of 9.525 mm and a wall thickness of 1.65 mm. The measured data were compared with the Dittus–Boelter correlation which showed 60% under prediction. Hoffman and Lones [4] conducted experiments on FLiNaK flowing in forced convection through circular tubes. The test section included 61-cm long tubes of nickel, Inconel, and Type 316 stainless steel. Each tube was long enough to allow fully developed flow. Twenty-four equally spaced thermocouples were used to monitor the outside surface temperature profile of the test section. Data obtained under predicted the Dittus–Boelter correlation by 60%. Vriesema [5] performed forced convection heat transfer experiment in a vertical test section of Inconel-600 alloy. The data obtained were compared with Dittus–Boelter correlation and it has under predicted by 15%. Ignat'ev et al. [6] have performed heat transfer studies using FLiNaK in a circular tube of iron based steel-Kh18N10T. The data were compared with the existing Sieder-Tate and modified Petukhov correlations. Heat transfer characteristics of molten salts depend on their thermo-physical properties. Table 2 summarises the properties of FLiNaK used in the former studies. Of the properties that were used in the experimental analysis, only the thermal conductivity values were considered to influence the heat transfer (Nusselt, Nu and Prandtl numbers, Pr) values. Previous researchers, Grele and Gedeon [3],Hoffman and Lones [4], and Vriesema [5], had used thermal conductivity values of 4.5, 4.5, and 1.3 W/mK, respectively. In order to test this possibility, Ambrosek et al. [7] have re-analysed each of these experiments with consistent and the most widely accepted values for the FLiNaK salt thermo-physical properties. They used three thermal conductivity values including correlation developed by Smirnov et al. [8]. The correlation is given below, $k = 0.36 + 5 \times 10^{-4}T$. Where, k is the thermal conductivity and T is temperature in Kelvin (K). Smirnov's correlation gives values ranging from 0.81 to 0.93 W/mK over a temperature range of 535 to 751 °C. The analysis of the experimental data using Smirnov et al. [8] correlation and a constant value of 1.0 W/mK for thermal conductivity, showed that the experimental heat transfer data over predicted the Dittus–Boelter correlation by 15%, for Reynolds numbers from 10,000 to 100,000.

Ferng et al. [9] have carried out CFD simulation of FLiNaK using standard $k-\varepsilon$ model. They validated the simulation results with the help of friction factor, Nusselt number, and hydraulic and thermal entrance length. They performed this analysis in a round tube of diameter 0.17 cm and length 15 cm. These experiments were performed at various Reynolds numbers in the range of 10^4 to 10^5. The inlet temperature was 500 °C with an input heat flux of 1.4 MW/m^2. The predicted fully developed friction factor corresponds well with that calculated by Blasius correlation and Moody diagram. Predicted Nusselt number also showed good agreement with the previous known correlations.

2.2. Flow structure identification and characterisation

Flow structures within the process equipment are the characteristic features of the local turbulence and play an important role in governing the transport phenomena. Turbulent flow parameters like eddy age distribution, turbulent kinetic energy, characteristic

Table 1
Summary of experimental heat transfer investigations of FLiNaK.

Sr No	Experimental details	Reynolds number	Prandtl number	Advised correlation	Reference	Deviation from compared correlation
1	Forced convection experiment in Inconel X test section $D = 0.6223$ cm $T_{fluid} = 540–729$ °C Heat flux = 28–606 kW/m^2 Horizontal heating	2000–20000	5.2–15.6	Dittus Boelter	Grele and Gedeon [3]	Dittus–Boelter, 60% deviation
2	Forced convection heat transfer experiment in a circular tube in Inconel, Nickel, SS-316 alloy pipes $D = 0.4445, 0.2985, 0.4572$ cm $T_{fluid} = 646–702$ °C, 527–734 °C, 722–745 °C respectively for each pipe alloy Heat flux = 29–540, 73–604, 252–381 kW/m^2 Horizontal heating	2800–9500	4.9–17.1	Dittus Boelter (Colburn)	Hoffman and Lones [4]	Dittus–Boelter, 60% deviation
3	Heat transfer experiment in vertical test section of Inconel 600 alloy $T_{fluid} = 575–675$ °C Vertical cooling	14000–93000	6.9–12.3	Dittus Boelter	Vriesema [5]	Dittus–Boelter, 15% deviation
4	Heat exchange experiment in a circular tube of iron based steel-Kh18N10T $D = 0.3$ cm $T_{fluid} = 550–650$ °C Heat flux = 30–60 kW/m^2 Vertical heating	5000–15000	1.7–2.3	Sieder–Tate, Modified Petukhov	Ignat'ev et al. [6]	Not reported in the literature
5	Data re-evaluation of previous experimental results	–	–	Dittus Boelter	Ambrosek et al. [7]	Dittus–Boelter, 15% deviation