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## Research Paper Reactive cooling simulation of electronic components



# Kai Zhang<sup>a,\*</sup>, Alpo Laitinen<sup>b</sup>, Yazhou Shen<sup>a</sup>, Ville Vuorinen<sup>b</sup>, Christophe Duwig<sup>a</sup>

<sup>a</sup> Department of Chemical Engineering, Royal Institute of Technology (KTH), Brinellvägen 8, 114 28 Stockholm, Sweden <sup>b</sup> Aalto University, Department of Mechanical Engineering, FI-00076 Aalto, Finland

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#### ABSTRACT

Low-grade heat recovery is an indispensable solution towards high energy efficiency of power electronics. The fast pace of sustainable digitalisation calls for developing alternative solutions to create a sustainable loop for decreasing the energy footprint. However, heat transfer under low-temperature differences challenges effective heat recovery processes. Therefore, in this paper, reactive fluid performance in a practical heat exchanger is investigated using high-fidelity finite rate chemistry method, which is a key step to deploy the attractive Ericsson cycle for low-temperature heat-to-electricity conversion. Under fixed thermal efficiency, it is found that replacing non-reactive fluid by  $N_2O_4$  reactive fluid can immediately boost electrical efficiency of an Ericsson cycle by at least 260%. The needed primary heat exchanger component in an integrated cooling and power electronic system can be 54.8% smaller in volume whilst enabling a 26% higher thermal performance, provided that the hot source temperature is low (<403 K). For thermal processes involving high temperature hot source, substantial limitation of chemical reaction rate on the effectiveness of an Ericsson cycle is identified. Remarkably, low temperature difference is not a limitation for reactive heat transfer that continuous endo-/exothermic reaction happening throughout a heat exchanger improves Nusselt number Nu = 7.5 by a factor of ~ 1.3 than the corresponding value (Nu = 5.9) for non-reactive fluid. Turbulence is found beneficial for reactive heat transfer, suggesting the use of corrugated-type heat exchangers for better thermal exchange rates.

#### 1. Introduction

#### 1.1. Energy consumption in digitalisation and other industries

The digital transformation of our society calls for higher energy consumption year-by-year for data storage and computing. In 2021, the global electricity demand for data centres was approximately 220-320TWh that excluding the costly energy use for cryptocurrency mining, this was around 0.9–1.3% of global final electricity demand [1]. By 2030, it is anticipated that one-third of our total electricity demand in information and communication technology will be from data centres [2]. The major electricity consumption in data centres happens at different electronic components of servers, *e.g.*, processors, RAM sticks, *etc.* within which electricity turns to low-temperature heat. To avoid overheating, these devices must be cooled to operate, for example, at a temperature lower than 318 K for data storage devices and the RAMs [3]. The American Society of Heating, Refrigerating and Airconditioning Engineers suggests that a data centre operating at

291–300 K is needed to avoid the malfunction of major electronic components [4], though individual components may work well at higher temperatures, *e.g.*, up to 350 K.

In the context of rising electricity prices in Europe and the rest of the world [5], an integrated cooling and power electronic system (ICPES) capable of utilising coolant for power production is in high demand. The system increases energy consumption efficiency by creating a sustainable loop of "electricity - wasted joule heat (cooling) – electricity". This requirement is also vastly needed in many other high energy consumption industries such as the food and drink industry, chemical industry, glass industry *etc*, where low-grade heat utilisation has been one of the major challenges of the green transition. According to the evaluation of Forman *et al.* [6], nearly 72% of the world primary energy use is wasted, within which 63% are from the low-grade heat source with temperature below 100°C. In fact, one successful attempt to use waste heat from the data centre for power is made by Keskin and Soykan [7]. They showed that integrating combined cooling, heating and power system around the data centres can cut their annual operating cost by

\* Corresponding author.

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*E-mail addresses:* kaizhang@kth.se (K. Zhang), alpo.laitinen@aalto.fi (A. Laitinen), yashen@kth.se (Y. Shen), ville.vuorinen@aalto.fi (V. Vuorinen), duwig@kth. se (C. Duwig).



Fig. 1. Simplified schematic diagram of closed Ericsson cycle.

40.3%.

#### 1.2. Integrated cooling and heat recovery

Recently, Zhang et al., [8] reviewed state-of-the-art electronic cooling techniques. Common methods for electronic cooling are classified into direct and indirect methods. The former consists of air cooling, spray and jet impingement cooling, immersive cooling etc., and the latter uses microchannels, heat pipes, vapour chambers etc. filled with suitable coolants for effective cooling. For combined operation cooling and heat reuse, low-temperature district heating (LTDH) running on water is deemed an indirect cheap thermal management method in many sectors [9,10]. The latest review by Behzadi et al. [11] unravelled the potential of using liquid mediums for low-temperature heating (LTH) and high-temperature cooling (HTC) in combination with data centres. They highlighted the role of the liquid medium in providing not only cooling service but also heat storage in a thermal energy storage (TES) system. In this context, sensible heat storage in high heat capacity liquid and latent heat storage in liquid-gas phase change are the common choices [12,13]. The latter provides at least 5–10 times higher thermal energy storage, while the high-volume expansion during phase change was deemed a limitation for TES applications. Despite this, for combined operation cooling and power production, the Organic Rankine cycle (ORC) running on organic fluid, which relies on the concept of latent heat storage, benefits from the high-volume expansion [14,15]. In the past, the ORC cycle has received much attention attributed to its capability of extracting thermal energy from hot sources featuring temperatures as low as 80°C via fluid boiling [16,17]. Indirect contact with a hot source in the evaporator stores thermal energy in the form of latent heat, converted to mechanical energy in the expander, then condensed and pumped to the evaporator for completing the loop. According to Zhang et al. [8], other than using water and organic fluid as coolants, fluids such as nanofluids [18] and liquid metals [19,20] are promising candidates for indirect cooling and heat recovery.

Besides these choices, Behzadi et al. [11] discussed another very attractive TES method, namely the thermochemical energy storage using the reactive medium. Despite the almost highest energy storage density, the slow reversible reaction rate of reactive fluid limits the applicability of the method in, for example, the building environment. In this regard, N'Tsoukpoe and Kuznik [21] performed an in-depth analysis and highlighted the limitation of thermochemical heat storage for domestic applications due to the significant thermal loss. The promising aspect of this method was recognized as overestimated. Nevertheless, these drawbacks highlighted by Behzadi et al. [11] and N'Tsoukpoe and Kuznik [21] can become advantages if a fast enough reactant such as nitrogen tetroxide (e.g.,  $N_2O_4 \Rightarrow 2NO_2$  [22]) is screened out for effective cooling and for on-site thermal energy to electricity production rather than the TES. This introduces an alternative solution, other than the traditional ORC cycle, for combined operation cooling and power production. Moreover, such a fast reactant may offer an alternative energy

recovery strategy for the ORC cycle as well.

#### 1.3. Reactive fluid for power production and problem identification

Lasala *et al.* [23] investigated the concept of a thermochemical engine and extensively discussed the benefit of using reactive working fluid in closed gas power cycles. They reported that thermochemical engines can work efficiently in applications involving low-temperature hot sources or high-temperature cold sinks. Indeed, in closed gas power cycles, the thermochemical engine concept turns the conventional Brayton cycle into the idealised Ericsson cycle, as given in Fig. 1. A typical closed Ericsson cycle features the maximum power output by multi-stage intercooling compression and multistage reheating expansion attributing to the endothermic and exothermic reactions. In another attempt of using reactive fluid within the high temperature (~700°C) liquid/gas cycle, Binotti *et al.* [24] reported additional benefits of using N<sub>2</sub>O<sub>4</sub>/CO<sub>2</sub> blends than reactive N<sub>2</sub>O<sub>4</sub> fluid alone to improve the thermodynamic efficiency of solar power plant, attributing to the involvement of *iso*-thermal condensation process.

However, the main benefits of using reactive fluid for heat extraction have been largely ignored in these studies. That is, the true heat transfer capability of the reactive fluid is not investigated. As discussed by Zhai *et al.* [25], publications often focus on first-law efficiency to optimise cycles and select fluids. In the case of open-type heat sources, high efficiency can always be reached by increasing the  $T_{h1}$ , but it may result in a practically lower power heat source utilisation and hence a lower power output [26]. In essence, this means that without knowing how much heat can be extracted by a reactive fluid from a hot source, it is unclear whether the fluid will be useful for power production. For example, assuming one has optimised an open cycle with an efficiency of 100% (equivalent to the closed cycle definition given in Zhai *et al.* [25]), but the fluid can only extract the energy of 1 W out of the 1000 W 'waste heat', the actual power output will be too low and the actual waste out of the 'waste heat' is 99.9%.

From a fundamental perspective, reactive heat transfer (or reactive cooling of electronic components) outperforms non-reactive heat transfer because its rate of energy absorption/release is dependent on not only the temperature difference but also the heat/enthalpy flux. For a non-reactive fluid, a small temperature difference of 1°C can cause the rate of heat transfer to become infinitely small, unless a high coolant flow rate is used. For a reactive fluid, temperature drives the chemical equilibrium and dictates the enthalpy change. A high mass flow rate may therefore not pose a severe limit on the rate of heat transfer. In this regard, Zhang *et al.* [27] performed a direct numerical simulation using the finite rate chemistry method to examine the details of the near-wall performance of reactive  $N_2O_4$ . Compared to non-reactive gases, reactive flow at a frictional Reynolds number of 180 presents an enormous increase in heat transfer coefficient by 600%. This is accompanied by an increase of energy absorption by  $\sim$  17% across a 4.8 m channel. They reported that these merits are a result of the exothermic reaction at the cold channel core (initially at 30°C) and the endothermic reaction near the hot source (fixed at 130°C).

More importantly, they also reported that the progress variable, which defines the degree of chemical conversion is close to unity. It implies that the reaction rate is, in general, fast enough to compete with the fluid advection rate. A small heat exchanger running on reactive fluid will, in most cases, outperform a large heat exchanger running on non-reactive fluid. However, their work also indicates that the advection rate may put a limit on the full chemical conversion, and hence deteriorate the performance of reactive fluid heat transfer. To fully understand reactive heat transfer, it is of ultimate importance to always utilize/resort to a finite rate chemistry model which takes the local character of the chemistry properly into account. Based on our literature survey, the only previous work addressing finite rate chemistry is the study by Zhang *et al* [27]. In fact, we are not aware of any earlier studies investigating reactive heat transfer mechanism using detailed, finite-rate



Fig. 2. Heat exchanger used for cooling the electrical component. (P1-P7 are probe locations to track channel centre fluid behaviour).

numerical simulations. Three practical questions emerge from the previous research:

- Will reactive fluid perform equally well in a practical heat exchanger as in a simple channel?
- How does turbulent flow under flow transitions affect the reactive heat transfer in the practical heat exchangers?
- How much can reactive fluid contribute the achievement of high electrical efficiency in the future ICPES system?

Overall, the present work aims to call for the attention of chemical engineers to use chemical reactions in a smart way to harvest low-temperature heat (<100°C) from data centres, inverters, or other electrical units. The paper is structured as follows. In Section 1, we briefly introduced the concept of reactive heat transfer and its applications. In Section 2, the numerical setups for simulating the use of  $N_2O_4$  in a multichannel heat exchanger for power electronic cooling are presented. In Section 3, the concerns of chemical reaction time on reactive heat transfer performance and power cycle analyses are elaborated, followed by presenting the three-dimensional numerical results. Finally, in Section 4, some suggestions on how to use  $N_2O_4$  for power production in a Regenerative Ericsson Cycle are briefly presented in conjunction with a conclusion of the present work.

#### 2. Numerical setups and methodology

#### 2.1. Presentation of a Multi-Channel heat exchanger (HTX) geometry

Fig. 2 shows a model heat exchanger to be numerically studied in the present work. Experimental testing of the practical heat exchanger was

performed at Aalto university and the heat exchanger was numerically analysed using a conjugated heat transfer approach by Laitinen et al. [28]. In their work, 16 electric resistors, modelled as heat sources and are attached to the back of the heat exchanger, were water-cooled in the laboratory at atmospheric pressure (0.1 MPa). The heat exchanger features 20 channels with equal widths of 3.6 mm and heights of 5 mm. Fluid flows into the heat exchanger through a perpendicular pipe (10 mm in diameter), turning its direction at the plate towards positive Xdirection, followed by a U-turn to reverse the fluid flow in the outer 10 channels (five on each side of the inner). The inlet temperature  $T_c$  of cooling water was 300 K and the near-wall hot source temperature  $T_h$ was about 313 K. Thermal images at the back of the heat exchanger were measured using an infrared camera and the exact wall temperature distribution was predicted using the conjugated heat transfer method. According to Laitinen et al. [28], for water flowing at 2 L/min, the Reynolds number is 4960 at the heat exchanger inlet and the Reynolds number is  $925 \pm 100$  for the individual channels. The process corresponds to turbulent-laminar transition due to the forced change of flow direction by geometrical shape.

#### 2.2. Problem description and case setup

In this work, we choose to numerically investigate six cases as given in Table 1. Cases 1 & 2 use temperature profiles from the work of Laitinen *et al.* [28], mimicking their lab and numerical setups. Cases 3 to 6, of which one case uses incompressible, non-reacting fluid and three cases (increased Reynolds number) use compressible, reactive N<sub>2</sub>O<sub>4</sub> for cooling and heat recovery, assume a constant channel wall temperature  $T_w = 350K$ .

With a non-uniform wall temperature setting, in Fig. 3a, we show

Table 1	L
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Case settings for different working fluids.

Items	Volume flow rate	Inlet Velocity	Inlet Reynolds Number	Fluid temperature	Wall temperature	Wall temperature Profile	
Symbols	$\dot{Q}$ [L/min]	$U_{in} [m/s]$	Re	T [K]	$T_w[K]$	-	
Coool incommute into	0	0.4	-	200		-	
Case1 – incompressible	2	0.4	4960	300	$\max \sim 313$	Lattinen et al. [28]	
$Case2 - N_2O_4$	12	2.54	4960	300	max ~ 313	Laitinen et al. [28]	
$Case3 - N_2O_4$	6	1.27	2480	300	350	Uniform	
$Case4 - N_2O_4$	12	2.54	4960	300	350	Uniform	
$Case5 - N_2O_4$	24	5.07	9920	300	350	Uniform	
Case6 – incompressible	2	0.42	4960	300	350	Uniform	



#### (b) Role of uniform wall temperature settings (Case 6)

Fig. 3. Instantaneous fluid temperature and wall heat flux assuming (a) non-uniform and (b) uniform wall temperature in cooling and heat recovery for power electronics.

Table 2 Physicochemical properties of incompressible fluid and compressible  $N_2O_4$  gas at 303 K and 1 atm [29].

	Symbols/Units	Cases 1&6	Cases 2-5
	_	Incompressible	N2O4/NO2/N2
Mass Fraction	Y [-]	1	0.75/0.2/0.05
Density	$\rho [kg/m^3]$	997	2.84
Specific heat capacity	$C_p [J/(kg \bullet K)]$	4180	845.6
Thermal conductivity	$k [kg/(m \bullet s)]$	0.610	0.017
Kinematic viscosity	$\nu [m^2/s]$	$0.86 imes10^{-6}$	$5.1 imes10^{-6}$
Lewis number	Le [-]	1	0.87/0.85/0.6
Prandtl number	Pr [-]	5.85	0.72
Pre-exponential factor	$A[s^{-1}]$	-	0
Model constant	β[-]	-	$1.98\times10^{-17}$
Activation energy	$E_a$ [Cal/Mole]	-	12,849

that heat flux is always positive at the channel inlet irrespective of the fluid used for simulation (cases 1 & 2). This indicates an increase in the internal energy of the fluid. However, as the fluid flows downstream, the heat flux points outwards and becomes negative values, providing no cooling services. To maximise the exergy from a power electronic system, it is worth noting that the optimising the design of electronic components is very important that in practical applications, heat flux pointing out of the heat exchanger should be avoided. The observation in Fig. 3a explains why the fluid temperature increase reported by Laitinen *et al.* [28] is only about 13 K. With this low-temperature increase, electrical efficiency from a ICPES will be naturally low.

To mimic the practical cooling of design optimised electronic components, we focus on cases 3 to 6 assuming a practically higher and a uniform temperature  $T_w = 350K$  at the channel walls. As shown in Fig. 3b, this setting is useful in avoiding the problem of negative heat flux along the channel walls. As we employ adiabatic wall assumptions at the two ends of the heat exchanger, zero heat flux is imposed at the Uturn and inlet/outlet vertical pipes.

Table 2 shows the physicochemical properties of the two

 Table 3

 A Summary of numerical boundary conditions for Cases 3–6.

Inlet	Outlet	Inner and Outer Channel	U-turns
Y = const	$\frac{\partial Y}{\partial n} = 0$	$\left(\frac{\partial Y}{\partial n}\right)_{w} = 0$	$\left(\frac{\partial Y}{\partial n}\right)_{w} = 0$
$\frac{\partial P_{total}}{\partial n} = 0$	$P_{static} = const = 1 atm$	$\left(\frac{\partial P_{total}}{\partial n}\right)_w = 0$	$\left(\frac{\partial P_{total}}{\partial n}\right)_n = 0$
$U_x = U_z = 0,$ $U_y = const$	$\frac{\partial U}{\partial n}=0$	U = 0	$\boldsymbol{U}=\boldsymbol{0}$
T = const = 303K	$\frac{\partial T}{\partial n} = 0$	T = const = 350K	$\left(\frac{\partial T}{\partial n}\right)_{w} = 0$
	Inlet $Y = const$ $\frac{\partial P_{total}}{\partial n} = 0$ $U_x = U_z = 0,$ $U_y = const$ $T = const =$ $303K$	InletOutlet $Y = const$ $\frac{\partial Y}{\partial n} = 0$ $\frac{\partial P_{total}}{\partial n} = 0$ $P_{static} =$ $1atm$ $1atm$ $U_x = U_x = 0$ , $\frac{\partial U}{\partial n} = 0$ $T = const =$ $\frac{\partial T}{\partial n} = 0$ $303K$ $\frac{\partial T}{\partial n} = 0$	InletOutletInner and Outer Channel $Y = const$ $\frac{\partial Y}{\partial n} = 0$ $\left(\frac{\partial Y}{\partial n}\right)_w = 0$ $\frac{\partial P_{total}}{\partial n} = 0$ $\frac{P_{static}}{const} =$ $1atm\left(\frac{\partial P_{total}}{\partial n}\right)_w = 0U_x = U_z = 0,  \frac{\partial U}{\partial n} = 0U = 0U_y = const\frac{\partial U}{\partial n} = 0T = const =350K$

investigated fluids: the incompressible, non-reactive  $H_2O$  and the compressible, reactive  $N_2O_4$ . Water ( $H_2O$ ) is the most often used coolant for electronic cooling, and it is liquid status at the temperature of our interest. According to Zhang *et al.* [27], below 373 K, reactive  $N_2O_4$  shows much higher specific heat absorption capability than water, which is why ICPES using reactive fluid is preferred.

Specifically, for N<sub>2</sub>O<sub>4</sub>, the fluid has a boiling point of ~ 295 *K* at normal pressure (1 *atm*). At the heat exchanger inlet where fluid temperature T = 303K and pressure P = 1atm, the one-step reversible reaction  $N_2O_4 \neq 2NO_2$  constants ( $A, \beta$  and  $E_a$ ) [29] given in Table 2 decides the fluid's equilibrium composition. The mass fraction of N<sub>2</sub>O<sub>4</sub> and NO<sub>2</sub> is then 75% and 20% respectively. For numerical simulation to track the species transport, an inert species N<sub>2</sub> of 5% is added to the composition without changing the chemical equilibrium status. Detailed numerical boundary conditions are summarised in Table 3.

These settings are overall the same as the reacting flow simulation in Zhang *et al.* [27] where more details of the reaction properties are presented. Briefly speaking, the forward reaction of  $N_2O_4 \Rightarrow 2NO_2$  is an endothermic process and the backward reaction is an exothermic process. According to our hypothesis, close to a hot surface (T = 350 K in our simulation) of a pipeline (or channel), endothermic reactions of

 $N_2O_4 \rightarrow 2NO_2$  will cool the surface. In contrast, near the centreline and far from the wall, exothermic reactions of  $2NO_2 \rightarrow N_2O_4$  are considered to release heat. This repeating endo-*/exo*-thermic process in a pipeline help achieve efficient local heat exchange, enabling fluid temperature to rapidly increase at the hot source of a closed Ericsson cycle (where  $T_{w1} < T < T_{h1}$  refer to Fig. 1).

#### 2.3. Solver, Models, Mesh, and numerical discretisation

In the present work, a large eddy simulation of reacting flow (cases 2–5) is performed using a finite volume based in-house reactingFOAM solver enforcing low-Mach formulation [30]. Under this formulation, a reference pressure  $p_0$  is employed to update the mixture density  $\overline{\rho} = \overline{(p_0/RT)}$  where the *R*, *T*, and  $\rho$  are the specific universal gas constant, the mixture temperature, and the density respectively. The accuracy of the solver has been extensively validated against experiments and used for simulating reactive fluid under various conditions [27,30–33]. In the LES framework, we apply a low-pass filtering technique to separate large (resolved) and small subgrid-scale (SGS) turbulence. Invoking density-weighted averaging, the following equations are obtained from the Navier-Stokes equations,

$$\begin{cases} \frac{\partial\overline{\rho}}{\partial t} + \frac{\partial}{\partial x_{j}}(\overline{\rho}\widetilde{u_{i}}) = 0\\ \frac{\partial(\overline{\rho}\widetilde{u_{i}})}{\partial t} + \frac{\partial}{\partial x_{j}}(\overline{\rho}\widetilde{u_{i}}\widetilde{u_{j}}) = -\frac{\partial}{\partial x_{i}}\overline{p} + \frac{\partial}{\partial x_{j}}(\tau_{ij}) - \frac{\partial}{\partial x_{j}}\overline{\rho}(\widetilde{u_{i}}\widetilde{u_{j}} - \widetilde{u_{i}}\widetilde{u_{j}})\\ \frac{\partial(\overline{\rho}\widetilde{Y}_{k})}{\partial t} + \frac{\partial}{\partial x_{j}}(\overline{\rho}\widetilde{u_{i}}\widetilde{Y_{k}}) = \frac{\partial}{\partial x_{j}}\left(\overline{\rho}\overline{D_{k}}\frac{\partial\widetilde{Y_{k}}}{\partial x_{i}}\right) - \frac{\partial}{\partial x_{j}}\overline{\rho}(\widetilde{u_{i}}\widetilde{Y_{k}} - \widetilde{u_{i}}\widetilde{Y_{k}}) + \nabla \bullet J_{Y} + \overline{\omega}\\ \frac{\partial(\overline{\rho}\widetilde{h}_{s})}{\partial t} + \frac{\partial}{\partial x_{j}}(\overline{\rho}\widetilde{u_{i}}\widetilde{h}_{s}) = \frac{\partial}{\partial x_{j}}\left(\overline{\rho}\overline{\alpha}\frac{\partial\widetilde{h}_{s}}{\partial x_{i}}\right) - \frac{\partial}{\partial x_{j}}\overline{\rho}(\widetilde{u_{i}}\widetilde{h_{s}} - \widetilde{u_{i}}\widetilde{h_{s}}) + \nabla \bullet J_{h} + \overline{\omega}_{h} \end{cases}$$

$$(1)$$

Where the Favre filtered quantity is given with a tilted bar and an over-bar is used to denote spatial filtering, *i.e.*,  $\tilde{q} = \overline{\rho q}/\overline{\rho}$  and. The  $\overline{D_k}$  and  $\overline{\alpha}$  are the species' molecular diffusivity and thermal diffusivity respectively. Introducing the Lewis number *Le*, the  $\overline{D_k} = \overline{\rho}Le_k/\overline{\alpha}$  with  $Le_k = 0.62, 0.91, 0.94$  for *k* being the N<sub>2</sub>, NO<sub>2</sub>, and N<sub>2</sub>O<sub>4</sub> respectively. The shear stress  $\tau_{ij} = 2\mu \widetilde{S_{D_{ij}}} = 2\mu \left[\widetilde{S_{ij}} - 1/3tr(\widetilde{S_{ij}})\right]$  where the  $\widetilde{S_{ij}} = (\partial \widetilde{u_i}/\partial \widetilde{x_j} + \partial \widetilde{u_j}/\partial \widetilde{x_i})/2$  is the filtered strain tensor and *tr* denotes the trace operator applied to the tensor matrix. Hence, the  $\widetilde{S_{D_{ij}}}$  is equivalent to the deviatoric part of the filtered strain tensor. The definition of the two flux terms  $J_Y$  and  $J_Y$  can be found in Zhang *et al.* [27] with the enthalpy flux reformulated due to the use of Fick's law.

To close the sub-grid transport terms in equation (1), we write,

$$\overline{\rho}(\widetilde{u_{i}u_{j}} - \widetilde{u_{i}}\widetilde{u_{j}}) = \frac{2}{3}\overline{\rho}k_{sgs}^{'}\xi_{ij} - 2\mu_{sgs}\widetilde{S_{D_{ij}}}$$

$$\overline{\rho}(\widetilde{u_{i}Y_{k}} - \widetilde{u_{i}}\widetilde{Y_{k}}) = \frac{\mu_{sgs}}{Sct_{sgs}}\frac{\partial\widetilde{Y_{k}}}{\partial x_{i}}$$

$$\overline{\rho}(\widetilde{u_{i}h_{s}} - \widetilde{u_{i}}\widetilde{h_{s}}) = \frac{\mu_{sgs}}{Prt_{sgs}}\frac{\partial\widetilde{h_{s}}}{\partial x_{i}}$$
(2)

Note here the  $k'_{sgs}$  term is ignored in OpenFOAM environment because it is often much smaller than the  $\bar{p}$ . The  $\mu_{sgs}$  is the SGS turbulent viscosity and is calculated using a cubic root volume method as  $\mu_{sgs} = C_k \rho \Delta \sqrt{k_{sgs}}$ . The WALE (wall-adaptive local eddy viscosity, [34]) method is used to calculate the SGS turbulent kinetic energy  $k_{sgs}$ . Both turbulent Schmidt number and Prandtl number are assumed to be unity, same as that used in Fooladgar *et al.* [35] and Duwig *et al.* [36].

The species formation and the energy production terms in **equation** (1) are modelled as,

#### Table 4

A summary of physical time for reaching steady-state and performing statistical averaging.

Case No:	1	2	3	4	5	6
Volume flow rate	2	12	6	12	24	2
$\dot{Q}$ [L/min]						
Case starts time instance [s]	12	12	12	12	12	12
Residence time $\tau_{res,f}$ [s]	3	0.5	1	0.5	0.25	3
Steady-state time and averaging start	15	12.5	13	12.5	12.25	15
time instance [s]						
Statistical averaging time $\tau_{avg,f}$ [s]	6	1.0	2	1	0.5	6
Case end time [s]	21	13.5	15	13.5	12.75	21

$$\overline{\dot{w}_{k}(Y_{k},T)} = \kappa \dot{w}_{k}(\widetilde{Y}_{k},\widetilde{T})$$
$$\overline{\dot{w}_{h}} = -\sum_{k=1}^{N} h_{s,k} \times \overline{\dot{w}_{k}(Y_{k},T)} = -\kappa \sum_{k=1}^{N} h_{s,k} \times \sum_{i} \omega_{i}(\nu_{ki}^{'} - \nu_{ki}^{''})$$
(3)

The progress variable  $\omega_i = k_{f,i}[C_{N204}] - k_{r,i}[C_{N02}]^2$  with *i* being unity for single-step  $N_2O_4 \rightleftharpoons 2NO_2$ . The  $C_{N204}$  and  $C_{N02}$  are the species' molar concentration for  $N_2O_4$  and  $NO_2$ . In **equation (3)**, a segregation factor  $\kappa = 1$  is fixed, unlike in many previous works where  $\kappa$  is calculated using a partially stirred reaction network model [30]. The rationale behind this is that we have a well-mixed mixture of very thin reaction fronts. The SGS turbulence is hence unlikely to change the reaction front structure. Note that for large eddy simulation of the incompressible, non-reactive fluid (cases 1 & 6), a pimpleFoam solver extensively validated in Zhang *et al.* [27] is chosen. The only difference is that in the other work, the SGS term was not used, explicitly resolving all turbulent eddies across a very refined mesh.

In the present work, a hexahedral dominant mesh used is the same as the one in Laitinen *et al.* [28] where the fluid domain contains 10.9 million cells. The mesh sensitivity study was also reported in that study that in the channel region, the cell number along *Y*- and *Z*- direction is the same, *i.e.*,  $N_Y = N_Z = 28$  and  $N_X = 800$  along the streamwise *X*-direction (refer to Fig. 2). The NS equations are discretized using the 2ndorder accurate spatial (Gauss linear reconstruction of the fluxes at cell faces) and temporal (backward) schemes. A PISO algorithm starting with a momentum predictor step followed by four velocity correction steps using Poisson's equation is employed to satisfy continuity. The maximum local Courant-Friedrich-Levy number *Co* is set at 0.6 for both reactive and non-reactive heat transfer problems, with the time step automatically evaluated using *Co*.

#### 2.4. Flow residence time and statistical data collection

In Table 4, the flow residence time  $\tau_{res}$  for different cases vary due to their different volume flow rate  $\dot{Q}$ . To evaluate the  $\tau_{res,f}$ , the normalized T, defined as  $(T - T_{min})/(T_{max} - T_{min})$  is tracked at 7 probe locations (refer to Fig. 2). The results of cases 1 & 2 are shown in Fig. 4 and the rest are given in Appendix A. All our calculation starts at the time 12 s because the non-uniform wall temperature from Laitinen *et al.* [28] is taken at about this time instant. For cases 1 & 2, in Fig. 4, the flow reaches steady-state in approximately 3 s (to 15 s) and 0.5 s (to 12.5 s) respectively, hence the magnitude is chosen as the flow residence time  $\tau_{res}$ . In our work, all cases are first run for  $1\tau_{res}$  sufficient to reaching steady state, then averaged over another  $2 \times \tau_{res}$ . Note that in our initial test, the case 1 was run for a longer time to 24 s to ensure that statistical time-averaged results are independent.

#### 2.5. Parameter/variable definitions

In the present work, the performance of the fluid is primarily evaluated using the following equations:

The heat transfer coefficient is defined as,



Fig. 4. Examination of residence time for reaching steady-state, measured by probed temperature at 7 locations (Refer to Fig. 2).

$$h = \frac{\alpha_{eff} \left(\frac{\partial h_e}{\partial n}\right)_w}{T_w - T_{ref}} \tag{4}$$

Where  $\alpha_{eff}$  is the effective thermal diffusivity,  $T_w$  is the wall temperature, and  $T_{ref} = T_{in}$  with  $T_{in}$  being the fluid temperature at the heat exchanger inlet.

The Nusselt number is defined as,

$$Nu = \frac{hL_c}{k} \tag{5}$$

Where the characteristic length is given as  $L_c = 2wh_i/(w + h_i) = 4.2mm$  and the *k* is the thermal conductivity of the working fluid. For reactive simulation, thermal conductivity varies due to the decomposition and recombination of N<sub>2</sub>O<sub>4</sub>.

The surface averaged heat transfer coefficient and Nusselt number are then given as,

$$\overline{h} = \frac{\iint hdS}{S}, \overline{Nu} = \frac{\iint NudS}{S}$$
(6)

Where S is the effective surface area of HTX defined in the region where  $(T_w-T_b)/T_w>$  1%. The Reynolds number in the channels is defined as

$$Re_c = \frac{|u_x| \times D_{ref}}{\nu} \tag{7}$$

Where the  $D_{ref} = D_i$  at the heat exchanger inlet and  $D_{ref} = L_C$  within the channel. The friction factor is calculated only in the channel section to avoid difficulties in determining the length (see *l* in Fig. 2) of the flow path in a non-uniform structure as,

$$f_c = \frac{\Delta P}{l} \times \frac{2}{\rho \times |u_x|^2} \tag{8}$$

Where the  $\Delta P$  is taken at the two sides of the channel and is space-



(a) Formation of NO<sub>2</sub> following  $N_2O_4 \rightarrow 2NO_2$  and  $2NO_2 \leftarrow 2NO + O_2$ 



(b) Formation of N<sub>2</sub>O<sub>4</sub> via  $N_2O_4 \leftarrow 2NO_2$  and formation of NO via  $2NO_2 \rightarrow 2NO + O_2$ 

Fig. 5. Change of species' forward  $(\tau_{k,c}^{fw})$  and backward reaction time  $(\tau_{k,c}^{bw})$  at different temperatures and pressures (0D analysis).



Case 6: Incompressible fluid, 1atm, Re = 4960

Fig. 6. Time-averaged flow structure and temperature distribution in the heat exchanger.

averaged over the area of the individual channel. The  $\rho$  is the density of fluid mixtures.

To measure the thermal performance [37] of the heat exchanger, each case is benchmarked against incompressible case 6 as follows.

$$\eta = \frac{\overline{Nu}}{\overline{Nu_6}} \times \left(\frac{\overline{f_6}}{\overline{f_c}}\right)^{0.3} \tag{9}$$

Where subscript 6 refers to incompressible case 6.

#### 3. Results and discussions

#### 3.1. Zero-D characterisation of chemical reaction rate for reactive fluid

Before discussing the 3D physicochemical behaviours of reactive fluid in the heat exchanger application, we would like to investigate the rate of chemical reaction and to unravel the limits of the reactive heat transfer concept. Such an approach will offer deeper understanding on why we suggest using the chosen reactive fluid only in the low-temperature (<100°C) heat recovery application. It should be noted that there exists a 2<sup>nd</sup> step slow reaction  $2NO_2 \Rightarrow 2NO + O_2$  when the fluid temperature is higher than 403 K. To characterise chemical reaction rate, we define a reaction time for NO<sub>2</sub> following [31] as,

$$\tau_{k,c} = n_r \times C_{sum} / \left( \sum_{n=1}^{n_r} \nu_{k,r} R R_{k,r} \right) \tag{8}$$

where the denominator is given as the sum of the reactants/products stoichiometric coefficient  $\nu_{k,r}$  multiplied by the backward (bw)/forward (fw) rate of progress  $RR_{k2,r}$  for each reaction  $n_r$ . The total species concentration  $C_{sum}$  with a unit of *kmol* pre *meter cube* is evaluated from the ideal gas law.

To help understand Fig. 5, we would like to first highlight that for each subplot, (1) two vertical axes are used that the left and right axis each reflects the values of lines to the left and to the right of 403 K, (2) the right vertical axis uses log scale and the reaction time has a unit of milli-second.

As shown in Fig. 5a and 5b, forward  $(N_2O_4 \rightarrow 2NO_2)$  and backward reactions  $(N_2O_4 \leftarrow 2NO_2)$  have small time scales of  $O(\sim 10^{-5} \sim 10^{-4}s)$  (or smaller than 0.2 ms) for low-temperature applications with T < 403K. However, for high-temperature applications with T 700K, the backward recombination time to NO<sub>2</sub> via  $2NO_2 \leftarrow 2NO + O_2$  is at a scale of  $O(\sim 1s)$ (Fig. 5a, right half, where reaction time is  $10^3ms = 1s$  at T = 700 K). For the forward reaction decomposing NO<sub>2</sub> to NO via  $2NO_2 \rightarrow 2NO + O_2$ , the chemical time scale is unacceptably large, at a scale larger than O(10 s)(Fig. 5b, right half, where reaction time is  $10^4ms = 10s$  at T = 700 K). Although high pressure reduces the reaction time, the yet long chemical reaction time implies insufficient time for the endo-/exothermic reaction to happen in high-temperature applications. For instance, these observations imply that constructing high-temperature Ericsson cycle for thermal-to-electricity conversion may cause a looping system to end



Fig. 7. Contour of the time-averaged velocity and N<sub>2</sub>O<sub>4</sub> mass fraction fields for case 4 to demonstrate the impact of vortices.



Fig. 8. Nusselt number distribution across the heat exchanger.

up with a mixture of NO and  $O_2$ . The system fails unless a sufficiently big cooler is constructed to convert NO and  $O_2$  back to  $NO_2/N_2O_4$ , which is most likely impractical.

## 3.2. Time-averaged fluid characteristics at constant Reynolds number (LES)

Fig. 6 shows the time-averaged temperature contour inside the heat exchanger for cases 4 (compressible, reactive fluid) and 6 (incompressible, non-reactive fluid) as well as their associated line integral convolution (LIC) vector fields for clear visualisation. The two cases are chosen here for comparison because they share a same Reynolds number at the heat exchanger inlet. At a first glance, the inlet/outlet flow structures of two cases are very similar. In the inner channels of the heat exchanger, N<sub>2</sub>O<sub>4</sub> temperature increases rapidly in a very short distance while the incompressible fluid temperature remains nearly unchanged in this section. The notable incompressible fluid temperature increase only happens in the outer channel due to the short flow residence time of this case and the high heat capacity of the fluid. As a result, the incompressible fluid temperature at the heat exchanger outlet is about 20 K lower than the N<sub>2</sub>O<sub>4</sub> gas.

Besides, in Fig. 6, an abrupt temperature increase is observed for both cases at the immediate exit of inner channels. A closer look at the region in Fig. 7 shows that the temperature increase occurs at where flow separation leads to the formation of vortices. According to Laitinen et al. [28], the flow separation distributes the fluid momentum outwards, resulting in lower flow rates in channels #5 and #16 (see channel annotations in Fig. 7). The large primary flow structure denoted in Fig. 7 diverts the fluid towards the wall of the heat exchanger, resulting in larger flow rates in channels #1 and #20. These observations partly explain why high-temperature spots occur in the vortices. That is, the formation of these flow structures increases the flow residence time and disrupts the growth of the boundary layer, enabling heavy heat exchange between the cold core and hot near-wall fluids. Although the formation of longitudinal vortices is known as beneficial for heat transfer [38], vortex formation does not necessarily contribute to the overall heat exchanger performance because it also leads to increased pressure drop. This will be further elaborated in the present work. On the hand, the primary flow, as it has no direct contact with the hot source, we see in Fig. 6 that there is a temperature drop with its role in

heat transfer further discussed in the following.

To distinguish the fluids' different heat transfer mechanisms in the practical heat exchanger, time-averaged Nusselt number is chosen for providing a first insight into the fluid characteristics. In Fig. 8, the probability density function (PDF) plot shows that under the same inlet Reynolds number, the median Nusselt number for N<sub>2</sub>O<sub>4</sub> is about 7.5 and the incompressible fluid is 5.9. It indicates that for N<sub>2</sub>O<sub>4</sub> fluid, convection dominates strongly to the heat transfer. The high Nusselt number of the N<sub>2</sub>O<sub>4</sub> fluid is seen lasting longer across the inner channels that the fast temperature increase in the channel does not severely limit the convective heat transfer. Note that here we use equation (5) for calculating the Nusselt number which also reflects the change of local heat flux. In Appendix B, we provide the distribution of a local Nusselt number for all cases 3–6, where  $T_b$  is the bulk temperature along the channel length. The different definitions will only change the absolute value of the Nusselt number with the pattern of the curve remaining unaffected. For an integrated cooling and power electronic system, high Nusselt number of reactive than non-reactive fluid implies that the employed heat exchanger component can be smaller as we will prove in Section 3.4.

In addition, in Fig. 8, it is interesting to see that for both fluids, there is first a decrease of Nusselt number towards downstream, followed by an increase in the outer channels. This unique behaviour calls for extra attention in heat exchanger design. Apparently, the backward increase of the Nusselt number is associated with the formation of the primary flow structure denoted in Fig. 7. A significant increase of turbulent mixing (see Fig. 9) across the different fluid layers acts to lower the fluid temperature at the U-turn region (see Fig. 6). Again, at the U-turn, an adiabatic condition is applied on the wall, hence temperature should ideally remain unchanged. The promoted mixing of fluids is favoured in heat exchanger design, while the effect of primary flow on pressure drop must also be considered.

Fig. 9 shows that despite the same inlet Reynolds number of the two cases at the heat exchanger inlet, there are notable differences in the pressure drop rate (per meter) and turbulent intensity between different fluids. Here, the two quantities are defined as,

$$I' = \sqrt{\frac{\widetilde{u'u'}}{\widetilde{UU}}}, p = \left|\frac{\partial\widetilde{P}}{\partial X_i}\right|$$
(7)



(b) Pressure Drop

Fig. 9. Turbulent intensity (a) and pressure drop (b) across the heat exchanger.

Where the  $\tilde{q}$  refers to density-averaged quantity q.

For N<sub>2</sub>O<sub>4</sub>, it is found that turbulent intensity (Fig. 9a) is greatly amplified to be larger than 500% when the fluid impinges on the heat exchanger plate, while the intensity of incompressible fluid is much lower. Along the inner channels, both fluids show a decrease in turbulent intensity, indicating the flow laminarization. For both fluids, the turbulent intensity of the two most inner channels #10 & #11 (refer to channel number in Fig. 7) is, in general, higher than that in the two channels next. This non-symmetric turbulent intensity, which was also discussed in Laitinen et al. [28] is a result of the non-uniform inlet flow structure (refer to Fig. 6). At the U-turn downstream, it is interesting to see how N<sub>2</sub>O<sub>4</sub> quickly returns to very strong turbulent flow, while the turbulent intensity of incompressible fluid is lower. This is a very encouraging observation because the quick return to turbulent flow is often beneficial for heat transfer and the lower associated pressure drop rate (Fig. 9b) of reactive than non-reactive fluid is also desired. When fluid flows into the outer channels, increased turbulent intensity is also inherently related to the increased Nusselt number in Fig. 8, due to the promoted mixing of fluids' cold and hot layers.

3.3. Flow-turbulence interaction with heat transfer at constant Reynolds number

To examine the flow-turbulence interaction with heat release rate (*Qdot*) and local flux, normalised mutual information (MI) score is employed in Fig. 10 to find out their dependency on several instantaneous quantities (Q) [39]. The MI is defined in the way such that when MI score is zero, two chosen clustered quantities are independent to each other. When MI score is unity, the quantities are strongly dependent on each other. This investigation is applied to three parts of the heat exchanger due to the distinct flow behaviours: the inner channels where flow relaminarization occurs, the U-turn where strong turbulence intensity presents, and the outer channels where there is a backward increase of Nusselt number as a result of increased mixing in the U-turn.

In **Fig, 10**, the enthalpy gradients and heat flux are vector quantities. We use  ${}^{\prime}Q|Z'$  and  ${}^{\prime}Q|Y'$  to denote the magnitude of quantity *Q* along the spanwise *Z* and vertical *Y* directions respectively. The flow streamwise direction is denoted with Q|X. Focusing on the spanwise heat flux along the Z direction, in Fig. 10, we observe that,

• Spanwise heat flux (heat flux  $|Z\rangle$  always have the highest dependencies on enthalpy gradient |Z (MI = 1.0) because the two are



(c) Outer ChannelFig. 10. Mutual score between heat flux |Z and chosen quantities at different positions of the heat exchanger.

known linearly correlated. It evidences the effectiveness of the MI score in describing the dependencies.

- In the inner and outer channels, heat flux |Z| is found more dependent on reactive than non-reactive fluid properties, though the dependency is overall weak. The highest MI score, excluding the enthalpy gradient |Z| (MI = 1.0), is the heat release rate (for reactive fluid only), followed by enthalpy and temperature.
- In the U-turn, the MI score seems equally low for reactive and nonreactive fluid. It indicates that in this region, there must exist a drastic change in the heat transfer mechanism.

For ease of comparison, Fig. 11 shows the change of MI score at different positions of the heat exchanger for the reactive fluid and the non-reactive fluid separately. For reactive fluid in Fig. 11a, the dependency of heat flux |Z on the chosen quantities is the highest within



(a) Case 4: compressible  $N_2O_4 \rightleftharpoons 2NO_2$ , 1atm, Re = 4960





Fig. 11. Mutual score between heat flux |Z and chosen quantities for different cases.



Fig. 12. Cross-comparison of MI score (heat release rate verse chosen quantities) at different positions for case 4: compressible  $N_2O_4 \Rightarrow 2NO_2$ , 1 atm, Re = 4960.

the inner channels, decays in the U-turn, and then increases again in the outer channel. Interestingly, this observation agrees well with the change of Nusselt number in Fig. 8. It indicates that for reactive fluid, the Nusselt number change is mostly a result of coupled effect amongst

endo-/exothermic reaction, enthalpy, and temperature.

Similar observation also applies to non-reactive fluid in Fig. 11b, while the sensitivity of reactive fluid to the transition in and out of the U-turn region is clearly higher – the height of bar changes more for reactive



Fig. 13. Scatter plot of correlations between turbulent kinetic energy and the log10-based heat release rate/heat flux ( $Q = sign(Q) \times log_{10}(1 + |Q|)$ ).

than non-reactive fluid. It indicates that the strength of reactive heat transfer is more sensitive to the heat exchanger design (the sudden change of curvature or the flow transition).

To further explore the role of endo-/exothermic reaction on heat transfer, in Fig. 12, we report the MI score of heat release rate against several quantities for the reactive fluid only. In the U-turn region, the heat release rate has the highest dependency on the enthalpy gradient along the direction perpendicular to the heat exchanger plate, *i.e.*, the enthalpy gradient |Y. While in the inner and outer channels, the heat release rate has the highest dependency on the temperature, with its dependency on the enthalpy gradient reduced to about 1/3rd of that in the U-turn. The results seem very reasonable because, in the U-turn, the adiabatic wall assumption means that there is essentially no heat transfer from the wall. Local fluid properties such as enthalpy gradient drive the heat transfer and control the equilibrium status of reactive fluids. In the channel region, temperature is the main driving force for endo-/exothermic reactions to happen. Therefore, we may classify the channel and U-turn region into two different reaction regimes: the thermal runaway (temperature-controlled) and the radical explosion regime (species-controlled). It is also worth noting that for the radical explosion in the U-turn region, the heat release rate also has a high dependency on the turbulent kinetic energy, while the turbulence impact is again about 1/3rd in the channels.

Fig. 13 provides direct visualisation of the dependencies/correlations between turbulence and heat flux/heat release rate. Here, the heat flux or heat release rate is logged quantity, written as,  $Q = sign(Q) \times log_{10}(1 + |Q|)$  with *sign* being the sign function. Note that at the heat exchanger inlet, the compared two cases share the same fluctuation. However, in the inner channel, reactive fluid has already shown a larger fluctuation calling for extra attention in designing the inlet of a heat exchanger. At the U-turn, the turbulent kinetic energy increases, followed by a decay of turbulence in the outer channel.

Moreover, in the inner channel, we observe a double peak spanning from -5 to +5 for the heat flux. Although the flow rates of the compared two cases are very different, the absolute heat flux is similar. While, in the U-turn region, non-reactive fluid spans over a much larger heat flux range than that of the reactive fluid. The shrinkage of the reactive heat flux from [-5, 5] to [-2.5 to 2.5] seems to indicate that without any wall heat transfer, turbulence is easier to promote the thermal mixing of non-reactive than reactive fluid. This strengthened thermal mixing of incompressible fluid explains why in Fig. 8, the Nusselt number of incompressible fluid is higher for the fluid flowing into the outer channels. Nevertheless, we observe that for reactive fluid, many fluid parcels also feature low heat flux, *e.g.* from -1 to 1, where not many parcels exist for non-reactive fluid. This observation is a direct indicator of the existence of different heat transfer mechanisms that for reactive



Fig. 14. Instantaneous log10-based heat release rate ( $Q = sign(Q) \times log_{10}(1 + |Q|)$ ) at cutting sections of the heat exchanger. Row 1 at upstream and Row 3 at downstream (along X-direction).



Fig. 15. Change of Nusselt number, thermal performance, and friction factor over the inner channels.

Table 5			
A summ	nary of f	luid perf	ormance

Items	Inlet Velocity	Inlet Reynolds Number	Pressure Drop	Characteristic Volume	Friction Factor	Surface Averaged Nusselt Number	Thermal Performance
Symbols Units	$U_{in} [m/s]$	Re	$\Delta P[Pa]$	V [mm <sup>3</sup> ]	$f_c$	Nu	η
$Case3 - N_2O_4$	1.27	2480	8.4	3252.6	20.3	11.37	1.02
$Case4 - N_2O_4$	2.54	4960	31.8	3947.4	15.8	13.04	1.26
$Case5 - N_2O_4$	5.07	9920	90.8	7200	6.2	21.04	2.7
Case6 – incompressible	0.42	4960	212.6	7200	6.0	7.73	1

fluid, endo-/exothermic reaction happening throughout the heat exchanger (refer to 1st row of Fig. 13 where there is nearly no zero heat release rate) is responsible for heat transfer, hence enabling the occurrence of the low heat flux region. For non-reactive fluid, however, whenever the temperature gradient is low locally, no heat flux presents and therefore only high flux region exists (lack of low heat flux energy movement).

These observations indicate the stronger capability of reactive fluid in repeatedly absorbing and releasing energy even at low-temperature gradients. For non-reactive fluid, either high heat flux or no heat flux occurs, strongly limiting its performance in low-temperature waste heat recovery in, for example, a proposed power electronic system. The nonsensitive performance of reactive fluid to turbulence at U-turn (low mixing) suggests that turbulence generators are probably preferred in reactive heat transfer. For example, the use of a corrugated heat exchanger.

Finally, the endo-/exothermic reactions in the channel heat exchanger can be viewed in Fig. 14. Negative heat release rate close to the channel wall clearly indicates active absorption of thermal into chemical energy, and the positive heat release in the centre of the channel promotes local heat transfer. In addition, it is interesting to note that heat absorption reactions can also occur in the centre of the channel. They extend from the near-wall region as black spots to the channel centre almost in a continuous fashion. These are solid proofs for the occurrence of local non-equilibrium where mixing time is shorter than chemical reaction time. Repeately occuring of endo-/exothermic reactions are good signs of small heat exchangers showing outstanding heat recovery performance in a thermal-to-electricity conversion system.

#### 3.4. Cross-comparison of thermal performance for all cases

Fig. 15 shows the surface averaged Nusselt number  $\overline{Nu}$  (equation (8)) and the thermal performance  $\eta$  (equation (9)) for all cases. For reactive fluid, the  $\overline{Nu}$  if found to increase with Reynolds number *Re*. At the same *Re*, the  $\overline{Nu}$  for reactive fluid nearly doubles that of non-reactive fluid. Since  $\overline{Nu}$  is a surface-averaged quantity, it indicates the outstanding performance of reactive heat transfer on continuous heat absorption and surface cooling. Moreover, despite the high friction



Fig. 16. Energy change in the heat exchanger comparing outlet and inlet. (a) specific energy; (b) kinetic energy.

factor  $f_c$  of reactive fluid at Re = 4960, the thermal performance of reactive fluid is found 26% higher than the non-reactive fluid.

In Table 5, a summary of fluid performance is provided. Other than  $f_c$  and  $\eta$ , the characteristic volume is another useful metric to evaluate the fluid performance. It is defined as the required heat exchanger volume (or length since the cross-sectional area is fixed) for increasing the inlet fluid (coolant) from 300 *K* to 99% of the wall temperature (hot source), *i. e.*,  $T_b/T_w \approx 99\%$ . The faster the coolant reaches the highest possible temperature and the higher the fluid's Nusselt number, the more suitable the fluid may be useful for an integrated cooling and power electronic system (ICPES) as introduced in Section 1. At Re = 4960, we note that the characteristic volume needed for reactive fluid is 54.8% smaller than that of non-reactive fluid. Together with the doubled  $\overline{Nu}$  of reactive than non-reactive fluid, the outstanding thermal performance of reactive fluid is partly proven.

Of course, temperature can only reflect the change of sensible enthalpy  $(h_s)$ , while the enthalpy of formation or chemical energy  $(h^0)$ must also be considered when comparing reactive to non-reactive fluid. Therefore, in Fig. 16a, we report how specific energy ( $\Delta h_{se} = \Delta h_s +$  $\Delta h^0$ ) changes comparing the energy at the position where  $T_b/T_w \approx 99\%$ and at the inlet of the heat exchanger. For Re = 4960, the  $\Delta h_{se}$  for reactive fluid is about 2.6 times higher than non-reactive fluid. It indicates that for a power cycle with fixed thermal efficiency (since  $T_{h1} =$  $T_b \approx 99\% T_w$  is fixed, refer to Fig. 1), the electrical efficiency of ICPES using reactive fluid will be 2.6 times higher than using non-reacting fluid. In fact, with the same  $T_{h1}$ , the thermal efficiency of an Ericsson cycle running on reactive fluid can be significantly higher than the thermal efficiency of a Brayton (or Rankin) cycle running on nonreactive fluid, attributing to the reaction-enabled multi-stage intercooling compression and multistage reheating expansion [23]. In the end, the electrical efficiency of ICPES using reactive fluid may be 3 times higher than that of using non-reacting fluid. A complete cycle analysis based on the observations in the present work will be discussed in our future work.

Moreover, Fig. 16a shows that when *Re* increases from 2480 to 9920, the  $\Delta h_{se}$  has not changed much. This is because when  $T_b/T_w \approx 99\%$  is fixed, local fluids properties are nearly under equilibrium status, hence  $h_{se}$  is directly dependent on the local  $T_b$ . The observations in Figs. 15 and 16 indicate that N<sub>2</sub>O<sub>4</sub> is indeed a more suitable fluid for high-efficiency combined cooling and heat recovery.

Furthermore, since N<sub>2</sub>O<sub>4</sub> decompose into two NO<sub>2</sub> molecules under heat absorption, thermal expansion could lead to an increase in kinetic energy. It is therefore interesting to examine how the kinetic energy contributes to the total energy increase of the fluid using the definition  $\%\Delta KE = \Delta KE/(\Delta h_{se} + \Delta KE)$ . In Fig. 16b, as expected, incompressible fluid cannot expand via heat absorption, hence it generates an ignorable kinetic energy increase across the heat exchanger. While for N<sub>2</sub>O<sub>4</sub>, the increase of Reynolds number by 4 times from 2480 to 9920 increases the kinetic energy contribution to total energy by 19.6 times, though the absolute contribution of kinetic energy to total energy is low.

#### 4. Conclusions

In the present work, high fidelity, finite-rate numerical simulation of a channel heat exchanger filled with reactive fluid N<sub>2</sub>O<sub>4</sub> is performed for the first time. The aim is to call for the attention of chemical engineers to use chemical reactions in a smart way to harvest low-temperature heat (<100°C) from data centres, inverters, or other electrical units. In particular, the present work has practical implications for using Ericsson Cycle to cool and power electronic system for sustainable digitalisation.

First, we argue that the reactive fluid N<sub>2</sub>O<sub>4</sub> is more suitable for power electronic system involving low-temperature thermal to electricity conversion with hot source temperature T < 403K. Finite rate chemistry is identified as the main limitation for using N<sub>2</sub>O<sub>4</sub> reactive fluid in high temperature applications where *T* 700*K* and where the rate-limiting step

of  $2NO_2 \rightarrow 2NO + 2O_2$  has a time scale of order O(10 s). At low temperature, thermal to chemical conversion happens at a time scale of  $O(10^{-5} \sim 10^{-4}\text{s})$  benefiting the construction of efficient Ericsson cycle in ICPES invoking fast reversible reaction of  $N_2O_4 \approx 2NO_2$ .

Second, comparing reactive to non-reactive fluid, the key flow domain of the heat exchanger shows drastically different heat transfer mechanisms. Three flow domains are summarised for fluid flow in the investigated heat exchanger: (1) the inner channels where flow relaminarization is observed, (2) the U-turn where strong turbulence intensity presents, and (3) the outer channels where there is a backward increase of Nusselt number as a result of increased mixing in the U-turn. Using a mutual information score method for heat transfer analysis, we find that:

- In the inner (channel numbers: #6 to #15) and outer channels (channel numbers: #1 to #5 and #16 to #20), spanwise heat flux is dependent on primarily the reactive fluid properties such as the heat release rate, followed by enthalpy and temperature.
- The relative benefit of turbulence generation to heat transfer intensification may be significantly higher for reactive than for nonreactive fluid. With relevance to the present heat exchanger, this is noted in the U-turn region.
- It is reasonable to classify the channel and U-turn regions into two different reaction regimes: the thermal runaway (temperaturecontrolled) and the radical explosion regime (species-controlled) respectively. For radical explosion in the U-turn region, the heat release rate also has a high dependency on the turbulent kinetic energy, while the turbulence impact in the channel is less influential.

These observations call for the use of, for example, the corrugated heat exchanger for heat transfer intensification in future ICPES system. Turbulence carried reactive heat transfer has practical implications on enlarging the amount of heat recovered from electronic components that are attached to the surface of heat exchanger.

Third, the thermal performance of reactive fluid outperforms the non-reactive fluid in terms of sustainable heat absorption and heat release. At constant Reynolds number, reactive fluid presents a median Nusselt number Nu = 7.5 which is higher by a factor of  $\sim$  1.3 than the corresponding value (Nu = 5.9) for non-reactive fluid. The high Nusselt numbers of reactive fluid span over a large area of the heat exchanger even when the temperature gradient is low. The associated, continuous reversible reaction is found beneficial for the achievement of the high Nusselt number. For non-reactive fluid, however, temperature gradient significantly limits the heat transfer.

Overall, the present work demonstrates that  $N_2O_4$  is an attractive working fluid for constructing an integrated cooling and power electronic system capable of utilising coolant for low-temperature waste heat recovery and power production from electronics. For a power cycle to work under fixed thermal efficiency, reactive fluid can boost its overall electrical efficiency by at least 260%. Attributing to continuous low heat flux heat transfer at low-temperature differences, the needed primary heat exchanger component can be 54.8% smaller in volume whilst enabling a 26% higher thermal performance.

#### CRediT authorship contribution statement

Kai Zhang: Methodology, Formal analysis, Investigation, Writing – original draft, Writing – review & editing. Alpo Laitinen: Methodology, Writing – review & editing. Yazhou Shen: Writing – review & editing. Ville Vuorinen: Methodology, Writing – review & editing. Christophe Duwig: Methodology, Conceptualization, Writing – review & editing, Supervision, Funding acquisition.

#### **Declaration of Competing Interest**

The authors declare that they have no known competing financial



Fig. A1. Examination of residence time for reaching steady-state, measured by probed temperature at 7 locations (Refer to Fig. 2).



Fig. B1. Distribution of the local Nusselt number along the heat exchanger channel.

interests or personal relationships that could have appeared to influence

#### Appendix A

Fig. A.1. shows the time history of the normalised T at 7 probe locations. The data was used to monitor the residence time for a typical case to reach steady state. For all cases, two residence times are chosen for statistical data averaging.

#### Appendix B

Fig. B.1. shows the distribution of the local Nusselt number  $(Nu_L = Nu \times (T_w - T_{in})/(T_w - T_b)$  for all cases 3–6, where  $T_b$  is the bulk temperature along the channel length. The local Nusselt number differs from the Nusselt number given in **equation (5)** by changing only the magnitude. The pattern of the curves will remain roughly unaffected. In Fig. B.1., there is always a decrease in the Nusselt number downstream, followed by a sudden increase in the outer channels as a result of intensified mixing in the U-turn region of the heat exchanger. In all cases, the Nusselt number of compressible, reactive fluid is much higher than the incompressible, non-reactive fluid.

the work reported in this paper.

#### Data availability

Data will be made available on request.

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#### K. Zhang et al.

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