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Fully electrified heat pump assisted distillation process by flash vapour circulation

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ABSTRACT

In industrial processes there are instances where heat pump assisted distillation falls short of full electrification, necessitating an auxiliary reboiler. To solve this limiting issue, this short communication proposes a new method using flash vapour circulation (FVC) to recuperate the waste heat within the heat pump cycle. This method incorporates a flash drum after the throttling valve to generate flash vapour. Rather than employing an auxiliary cooler for condensing the mixed vapour-liquid in a conventional heat pump system, the produced flash vapour is circulated back to the compressor inlet to enhance the recycled heat in the reboiler. With proper energy match, this approach has the potential to realise full electrification of distillation. The distillation of methanol/water serves as an illustrative case study, showcasing the viability of FVC which allows additional 22% energy savings, as compared to mechanical vapour recompression. Yet, this strategy may not be advantageous if the waste heat is already maximally utilised in preheating both the compressor and column inlet feed. The separation of tetrahydrofuran/water is used as case study to demonstrate the limitations of this approach.

1. Introduction

Distillation is traditionally an energy-intensive thermally-driven separation process. To reduce the energy usage and achieve process decarbonization, electrification strategies such as mechanical heat pump assisted distillation have been widely used (Cui et al., 2020; Kiss et al., 2012; Kiss and Smith, 2020). Mechanical vapour recompression (MVR) is a prominent technique in this domain, especially for separating components with close boiling points (Cui et al., 2017; Fonyo et al., 1995), as illustrated in Fig. 1**a**. In such a system, the overhead vapour is used as heat storage and transfer medium, being compressed to a higher temperature and allowing its latent heat to be utilised in the reboiler. The high-pressure condensate is then expanded through a throttling valve to provide reflux and distillate. It is important to note that an additional heater (indicated by discontinuous lines) may be necessary to prevent liquid droplets from forming inside the compressor.

Occasionally, the compressed overhead vapour may not supply adequate heat for reboiler energy requirements. In such instances, an auxiliary reboiler may be necessary to compensate the energy deficit, thus a complete electrification (without use of steam) cannot be achieved. To address this issue, a flash drum can be placed after the throttling valve as demonstrated in Fig. 1**b**. This arrangement allows the flash vapour to be circulated either back to the compressor inlet or into the distillation column, increasing the vapour throughput in the compressor and thus generating more high-grade heat in the reboiler. The concept of flash vapour circulation (FVC) was previously introduced by Modla and Lang (2017). However, their original process lacked a cooler after the throttling valve, limiting the adjustments in vapour circulation flowrate to manipulating the compressor power. This concept was further extended by Ferchichi et al. (2022) and Hegely and Lang (2023), who added a cooler post-throttling valve, providing an additional variable to adjust the vapour circulation flowrate. The authors introduced a parameter β, representing the ratio of the flowrates of the compressing working fluid and the top vapor, to characterize the structure of the vapour recompression scheme. A value of β=1 indicates conventional MVR, β>1 means recirculation, and β<1 denotes bypassing the compressor. Given that this short communication primarily addresses scenarios where the condenser duty is less than the reboiler duty, the

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compressor bypassing method is out of scope.

It should be noted that the basic FVC structure (Fig. 1**b**) may require cooling of the post-expansion stream. As the expanded stream typically exhibits a lower temperature, its contained energy, whether latent or sensible, could be lost through the use of cooling water (CW). To exploit this potential waste heat, this short communication introduces a new FVC structure, as illustrated in Fig. 1**c**. An additional cooler is strategically placed before the throttling valve, allowing for the flexible adjustment of the desired vapor fraction while also facilitating waste heat recovery. The next section presents a case study about methanol/water distillation to demonstrate the benefits of the proposed FVC structure. It is also important to acknowledge that this method is not universally applicable, as demonstrated by a case study on tetrahydrofuran/water separation, which highlights the limitations of this approach. Notably, the aim of this short communication is to serve as a conceptual starting point, helping readers quickly recognize the existence and potential usability of the FVC structure. Further discussion about the applicable scenarios of FVC and other extensions will be considered in future research papers.

2. Case studies

2.1. Methanol/water distillation

The methanol/water distillation column has been adapted from the syngas-produced methanol flowsheet presented by Luyben (2010). Only considering the main components of the methanol/water feed, their molar concentrations are 0.8/0.2. Additionally, the feed flowrate is set at 100 kmol/h, with the feed temperature and pressure of 30 °C and 5 bar, respectively, considering the upstream fluid transport pressure. The distillation column has a total number of 40 stages (the 1st stage is the condenser and the 40th stage is the reboiler). The feed stage is the 30th stage. The condenser pressure is set at 1 bar, and a reasonable stage pressure drop of 0.7 kPa is assumed (Luyben, 2013). The methanol and water mole purity are set as 99 mol% and 99.99 mol%, respectively. Using Aspen Plus v8.8 with NRTL as suitable property model, the simulation results from the RadFrac module yield the solution through the "*Design Specification*" function. The reflux ratio is determined to be 0.645, while the condenser and reboiler duties are calculated to be 1307 kW and 1426 kW, respectively. The overhead vapour has a temperature of 64.8 °C, while the bottom temperature is 106.5 °C. Notably, the system is not further optimized since the focus of this paper is to propose the FVC structure.

In simulating the MVR and FVC configurations, the isentropic compression based on ASME method is used for the compressor settings and the isentropic efficiency is set at 0.75, as described in Kazemi et al. (2018). Within the heat pump systems, multiple compressors in series with intermediate heat exchangers are used to reduce compressor energy consumption and to keep the discharge temperatures in check (Luyben, 2011). For conservative design, the compressor discharge temperature is limited to 150 °C – for safety reasons, since at higher temperatures the system may fail from worn rings, acid formations and oil breakdown (Luo et al., 2015) – by adjusting the corresponding compression ratio (CR) and the temperature approach in heat exchangers is 10 °C. Notably, the specific limit temperature may depend on the compressor type, the compressed gas, and other factors. The pressure drops in both heat exchangers and flash drum are neglected for simplicity, as they are typically rather small.

The application of the MVR is given in Fig. 2, which involves a configuration with three compression stages using three compressors and two intermediate heat exchangers. This design takes into account the limitation on discharge temperature. It is important to highlight that the heat from these intermediaries is utilised sequentially to vaporize the liquid at the bottom of the column. The total compressor work is 287 kW, which is capable of upgrading 1325 kW of high-grade heat to drive the distillation column. Consequently, the coefficient of performance (COP) of the heat pump is 1325/287 = 4.617. The necessary reboiler duty for the distillation is 1426 kW, leading to an energy deficit of 101 kW for the separation. Therefore, additional energy input from low-pressure steam (LPS) via an auxiliary reboiler is necessary, bringing the total energy requirement to 287 + 101 = 388 kW. In the MVR system, the vapour fraction of the stream after the throttling valve is 0.2057 with a temperature of 64.55 °C. Given this temperature is typically too low for further use in chemical plants, CW is required to saturate (condense) the vapour-liquid mixture, inevitably degrading 268 kW of energy.

Considering the limitations of fully electrifying the MVR process, Fig. 3 introduces the FVC method as a means to achieve a complete process electrification. We consider this design as the FVC-1 configuration. In the current scenario, the FVC requires a total of 358 kW for compression, which is marginally lower than the 388 kW energy requirement observed in the MVR system. Notably, the FVC approach can entirely cover the reboiler duty of 1426 kW. Under these conditions, the COP for the FVC system is 1426/358 = 3.983, which is somewhat lower than that of the MVR system. However, the FVC generates 237 kW of waste heat at a considerably higher temperature of approximately 120 °C, making it viable for onsite reuse through methods such as heat integration, steam generation, or even power generation via an organic Rankine cycle (Li et al., 2019). In the FVC system, the overhead vapour flow from distillation column is 132.943 kmol/h, while the recycle flash vapour flowrate is 32.495 kmol/h, resulting in a recycle ratio of 32.495/(132.943+32.495) = 0.1964. This ratio can be adjusted by manipulating the waste heat duty. For example, the present results are calculated based on the condition that the cooler outlet is a saturated liquid. Altering this condition to achieve subcooling reduces the generation of flash vapour, thereby lowering the recycle ratio. Table 1 illustrates how varying degrees of subcooling impacts other system parameters. With the increase of the degrees of subcooling, the waste

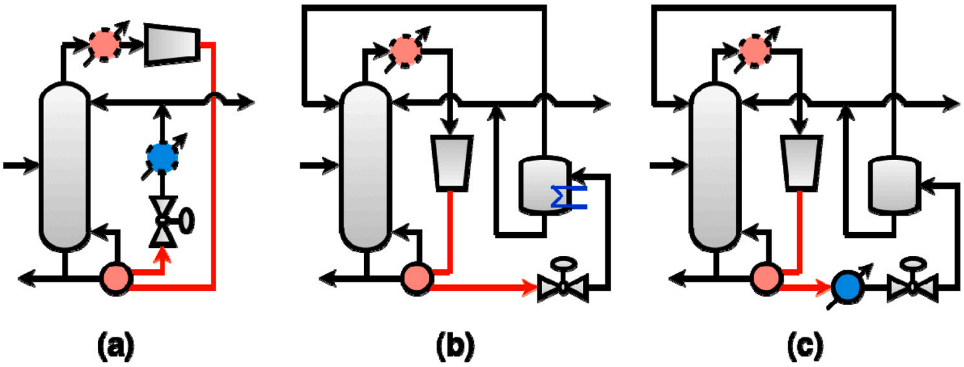

Fig. 1. (a) Mechanical Vapour Recompression (MVR), (b) MVR combined with Flash Vapour Circulation (FVC) adapted from Modla and Lang (2017) and Ferchichi et al. (2022), and (c) New structure of MVR-FVC.

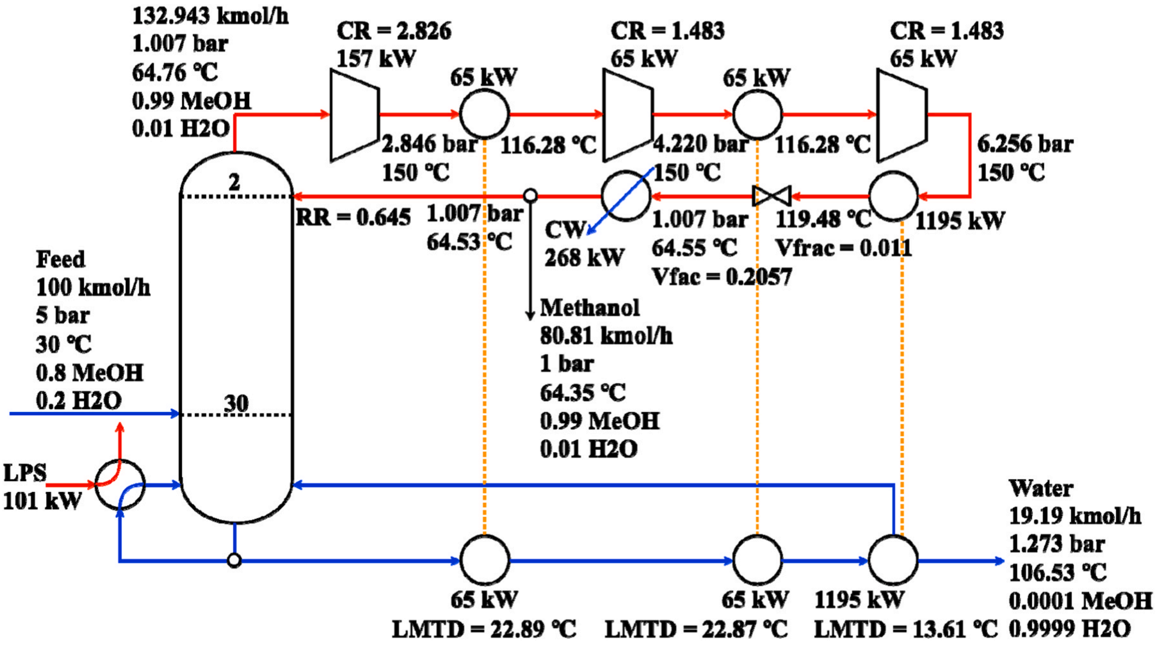

Fig. 2. MVR for methanol/water distillation.

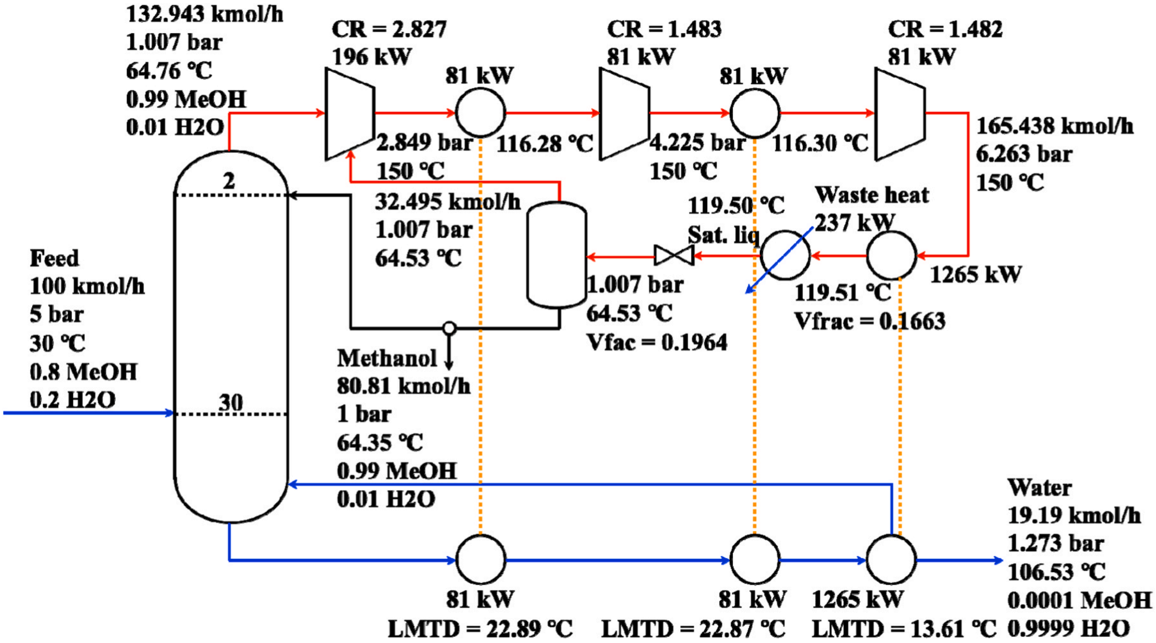

Fig. 3. FVC-1 for methanol/water distillation (cooling down to saturated liquid).

heat duty and total compression duty are decreased due to the diminished flow of recycle vapour. Additionally, this leads to an improvement in the COP, beneficial for enhancing the efficiency of the heat pump cycle. It is noteworthy that the maximum subcooling degree achievable in this context is 39 °C, beyond which a temperature crossover in the reboiler might occur, given that the minimum temperature approach is set at 10 °C.

To demonstrate the advantages of cooling the stream beyond its dew point, Fig. 4 presents the simulation results for the highest levels of cooling below the dew point, referred to as the FVC-2 design. This FVC-2 setup is entirely powered by electricity, with the total power required for compression being 302 kW. When compared to the MVR configuration, FVC-2 achieves energy savings of 22%. Furthermore, its COP is 4.722, surpassing that of the MVR process. Investigating why subcooling outperforms maintaining the saturated liquid reveals intriguing insights. In the MVR system, the distillate stream leaving the main reboiler has a vapour fraction of 0.011, indicating that approximately 99% of the latent heat has been utilised for boiling. Conversely, in the FVC-1 scheme, this vapour fraction is 0.1663, which indicates under-utilisation of the latent heat and consequent energy inefficiency due to the excessively high recirculation flowrates used for heat transfer. However, with adequate cooling as seen in FVC-2, this vapour fraction can reach as low as zero, indicating full utilisation of the latent heat. It is noteworthy that the waste heat in FVC-2 is in the form of sensible heat, which can be utilised to preheat the feed to the column. This approach of employing both latent and sensible heat, supplemented by mechanical

Table 1
Effect of the degrees of subcooling on other process parameters.

Degrees of subcooling (°C)	Cooling duty (waste heat) (kW)	Total compression work (kW)	Recycle flash vapour flowrate (kmol/h)	Recycle ratio	COP
0	237	358	32.495	0.1964	3.983
5	228	349	28.492	0.1765	4.086
10	220	341	24.757	0.1570	4.182
15	213	333	21.271	0.1379	4.282
20	206	327	18.004	0.1193	4.361
25	199	319	14.939	0.1010	4.470
30	193	314	12.064	0.0832	4.541
35	187	307	9.356	0.0657	4.645
39	183	302	7.303	0.0521	4.722

or electrical work, aligns with the concept of self-heat recuperation technology (SHRT) proposed in literature, as detailed in several studies (Kansha et al., 2009; Matsuda et al., 2011). However, it should be noted that the FVC method becomes redundant if the waste heat is already optimally utilised within the distillation system, as illustrated in the scenario described in the next section.

2.2. *Tetrahydrofuran/water distillation*

It is critical to understand that the FVC method is not universally applicable. The essence of FVC lies in the recovery of waste heat within the heat pump cycle. This determination may be made at the MVR application stage. During this stage, the user can assess the amount of waste heat in the condenser and determine if the FVC method can be effectively utilized. Should the waste heat be fully utilised elsewhere,

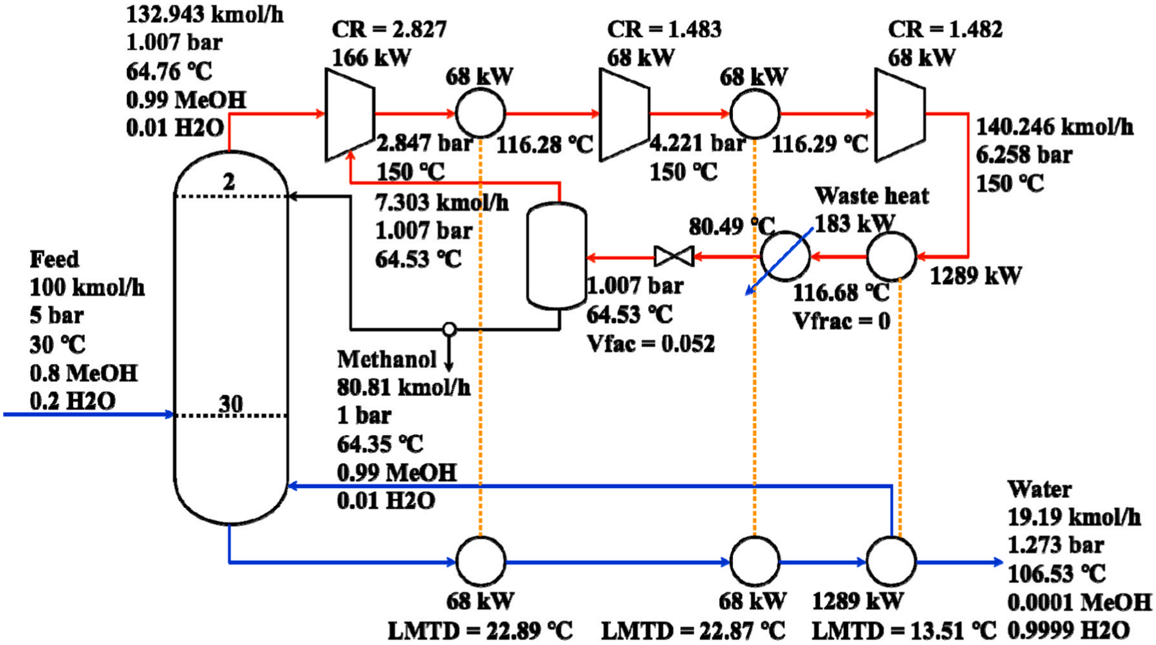

Fig. 4. FVC-2 for methanol/water distillation (cooling down to 39 °C of subcooling).

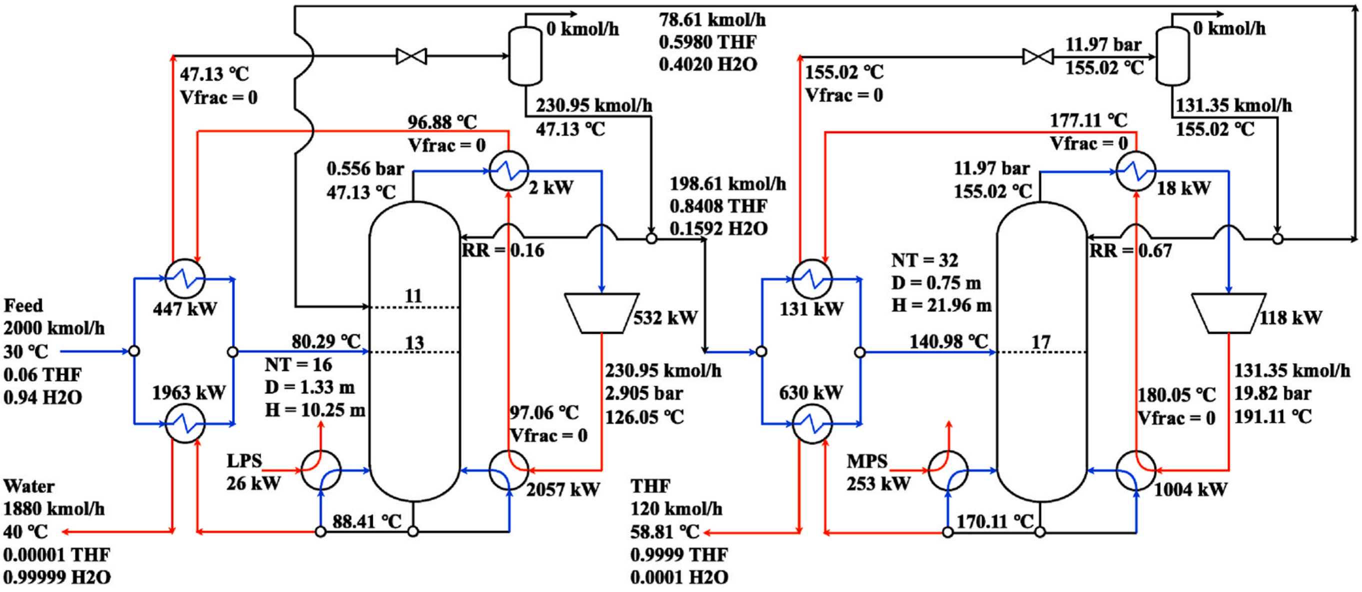

Fig. 5. SHRT for tetrahydrofuran/water distillation.

the FVC technique becomes inapplicable. To exemplify this limitation, an illustrative case study on tetrahydrofuran/water distillation is described here. Fig. 5 shows the optimum pressure-swing distillation process adapted from our previous study (Cui et al., 2020), where it is observed that in both distillation columns, the output steams from the main reboilers have a vapour fraction of zero, indicating complete utilisation of the latent heat. Additionally, the remaining sensible heat is employed for preheating both the compressor inlet and the column feed. After the throttling valve, there is no longer any flash vapour. Also, there is no need for an additional cooler to produce liquid distillate and reflux. However, the system still incorporates two auxiliary reboilers. Should the steam be produced via an electric boiler, the entire process could be considered electrified.

3. Conclusion

This short communication introduced an innovative approach to distillation, utilising FVC with heat pump assistance, and aiming at fully electrifying the process. The main concept of this technique involves recuperating the unused heat within the heat pump cycle by generating recycled flash vapour. A case study on methanol/water distillation demonstrates that the FVC can achieve additional 20% energy saving as compared to conventional MVR. Nonetheless, the applicability of FVC is limited in scenarios where the waste heat is already maximally leveraged, as showcased by the tetrahydrofuran/water distillation case study.

CRediT authorship contribution statement

Chengtian Cui: Conceptualization, Data curation, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. **Xiaodong Zhang:** Conceptualization, Data curation, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. **Hao Lyu:** Data curation, Investigation, Validation, Writing – original draft, Writing – review & editing. **Meng Qi:** Data curation, Methodology, Validation, Writing – original draft, Writing – review & editing, Investigation. **Anton A. Kiss:** Formal analysis, Investigation, Methodology, Supervision, Validation, Writing – original draft, Writing – review & editing. **Jinsheng Sun:** Conceptualization, Methodology, Supervision, Validation, Writing – original draft.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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