2024 PROJECT PEER REVIEW

U.S. DEPARTMENT OF ENERGY
BUILDING TECHNOLOGIES OFFICE

BTO Peer Review: Multiphysics Modeling of Heat Pumps

Multiphysics Modeling of Heat Pumps

Performing Organization(s): Argonne National Laboratory
PI Name and Title: Muhsin Ameen, Principal Research Scientist
Presenter Name and Title: Katherine Asztalos, Research Scientist
PI Email: mameen@anl.gov
WBS #: 3.2.2.63

Project Summary

OBJECTIVE, OUTCOME, & IMPACT

Objective: Leverage multi-fidelity simulations and HPC resources to model and optimize the performance of heat pump components
Outcome: Model-based design, improved accuracy of ROMs
Impact: Reduce cost and speed-to-market for low-GWP heat pumps

TEAM & PARTNERS

Microchannel condenser modeling
CRADA development with Rheem
Collaboration with Georgia Institute of Technology (Srinivas Garimella)
Multiple discussions with Oak Ridge National Laboratory (Kashif Nawaz & Bo Shen)

STATS

Performance Period: midFY23 – midFY26

DOE Budget: FY24: $500k

Cost Share: N/A

Milestone 1: CFD modeling of microchannel condenser

Milestone 2: Demonstrate impact of low-GWP refrigerants on condenser performance

Problem

Redesigning heat pump components for low-GWP refrigerants

- The buildings sector contributed an estimated 35% of total GHG emissions in 2021. Heat pumps with low-GWP refrigerants provide an efficient pathway towards decarbonizing HVAC
- There is a strong need to redesign heat pump components to:
  - Operate on low-GWP (<10) refrigerants
  - Have low-power requirements (compact)
  - Be efficient under challenging cold climate conditions
- Current best practices in heat pump design is to use simplified thermodynamic cycle analysis and 0D/1D simulations.
  - These studies neglect or simplify several key physics such as turbulent flow through expansion valves, phase change in evaporators and condensers, etc.
  - This can lead to heavy dependence on expensive experiments for generating data for the empirical models
- CFD tools that industry uses do not have all the necessary physics to perform predictive simulations
- **Goal:** Use CFD with accurate submodels to accelerate the design and reduce the cost of low-GWP heat pumps components to enable decarbonization goals

Problem

Redesigning heat pump components for low-GWP refrigerants

- The buildings sector contributed an estimated 35% of total GHG emissions in 2021. Heat pumps with low-GWP refrigerants provide an efficient pathway towards decarbonizing HVAC
- There is a strong need to redesign heat pump components to:
  - Operate on low-GWP (<10) refrigerants
  - Have low-power requirements (compact)
  - Be efficient under challenging cold climate conditions
- Current best practices in heat pump design is to use simplified thermodynamic cycle analysis and

> "Using CFD to optimize heat pump components can lead to a minimum improvement of **10% in COP** of the heat pump as the designed components will be better optimized " – Manager, HPWH OEM

- **Goal:** Use CFD with accurate submodels to accelerate the design and reduce the cost of low-GWP heat pumps components to enable decarbonization goals

Alignment and Impact

Alignment with BTO Blueprint

Alignment with BTO Crosscutting Goals

Prioritize equity – *Findings will be published in open literature so that the OEMs have access to the CFD findings to enable improving their 1D models.*

Prioritize affordability – *CFD simulations will help reduce the cost of developing new heat pump solutions with low-GWP refrigerants.*

Prioritize resilience

Alignment with BTO Strategic Objectives

Increase building energy efficiency – *Improving COP of heat pumps will lead to reduction in building energy use.*

Accelerate onsite emissions reductions – *Increased transition to heat pumps will accelerate on-site emissions reduction.*

Transform the grid edge at buildings

Minimize building life cycle emissions

Alignment and Impact

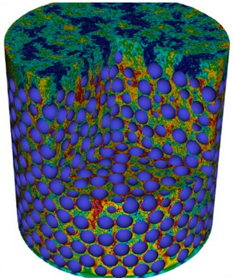
Deliverables and Impact

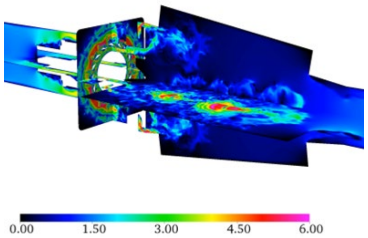
- **Project Deliverables:**
  - CFD models and dataset for components (evaporators, condensers, expansion valves, etc.), and refrigerants of high interest to industry
    - CFD simulations of microchannel condensers to evaluate impact of geometry and operating conditions (FY24)
    - First-of-its-kind fully-resolved CFD simulations of ejector heat pumps provide key insights (FY24)
  - Improved device-level correlations for low-GWP refrigerants developed based on the CFD dataset
  - Key findings on the sensitivity of geometric parameters on device performance for conventional and low-GWP refrigerants
    - CFD simulations of microchannel condensers with conventional and low-GWP refrigerants led to improved understanding of impact of refrigerant properties on device performance (FY24)
- **Impact:**
  - Reduce cost of heat pump design by reducing the number of experimental prototypes and measurements
  - Improve the accuracy of reduced order models used by the industry for heat pump design
  - Accelerate the heat pump design cycle (time-to-market)
  - Increased COP of heat pump due to optimized component designs

Approach

Leverage Core Capabilities in Exascale Computing and X-ray Science for HPs

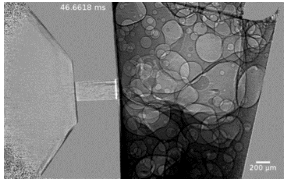
Exascale Computing using Nek5000[1]



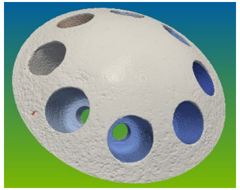


- One of the only high-order CFD codes that can handle complex geometries and run efficiently on GPUs
- Leveraging $15M+ ASCR investment and $7M+ EERE investment
- Demonstrated scalability up to ~30,000 GPUs.
- **Approach:** Exascale simulations deliver data-knowledge-tools to industry (models for heat transfer, phase change, etc.)

Advanced Photon Source Experiments



High-Speed Imaging of Flows Through Metal



High Precision Measurements of Flow Passages

- APS[2] is a national user facility housed at ANL providing ultra-bright, high-energy storage ring-generated x-ray beams for research in almost all scientific disciplines
- Facility is funded by DOE BES and has 5000+ users
- Demonstrated expertise in the team in using APS for multiphase flow measurements
- **Approach:** Utilize APS to perform in-situ, non-intrusive measurements in heat pump devices

[1] https://nek5000.mcs.anl.gov/

[2] https://www.aps.anl.gov/

Approach

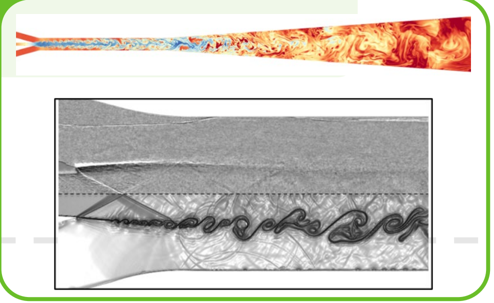
Multi-fidelity simulations to accelerate heat pump design

Improved CFD submodels

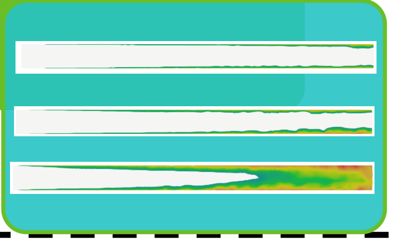
Device simulation data across a wide range

OEM Tasks

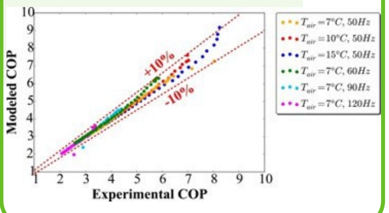
Highest fidelity interface-resolved DNS/LES



Device-level CFD using RANS/LES



Reduced order models



Argonne Tasks

- Utilize unique leadership computing resources and high-order CFD codes at ANL combined with X-ray and system-level experiments to accelerate design of heat pump components
- Multi-fidelity simulations have the potential to reduce time for moving from low-TRL to high-TRL

Partnership

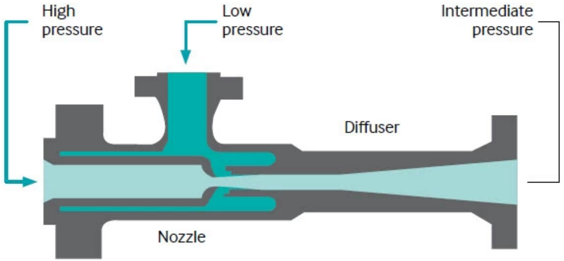
Experimental Measurements
- Device-level experiments (X-ray and lab-scale)
- Full heat pump experiments

Approach

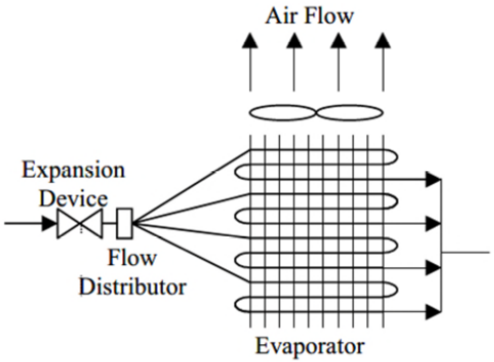
Demonstration Cases

- In current and near future, the multi-fidelity simulation approach is being demonstrated for 3 topics that are of key interest to the heat pump and heat pump water heater industries:
  - **Microchannel condensers (current)** – Use CFD simulations (validated with experiments from literature) to evaluate the impact of geometry, refrigerant properties, and operating conditions on condenser performance
  - **Ejectors for ejector-driven heat pumps (current)** – Use high-fidelity fully-resolved CFD simulations to model ejector-driven heat pumps and develop accurate reduced order correlations
  - **Distributors for evaporators/condensers (future work)** - Utilize a combination of high-fidelity CFD, high-fidelity X-ray visualizations leveraging the Advanced Photon Source (APS), and system-level experiments to minimize refrigerant maldistribution in heat pump evaporators to improve heat pump performance.

Image from "*Microchannel Coils Add Dimension for Cooling Systems*"



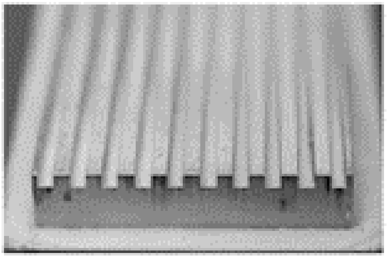
[1]https://www.ipieca.org/



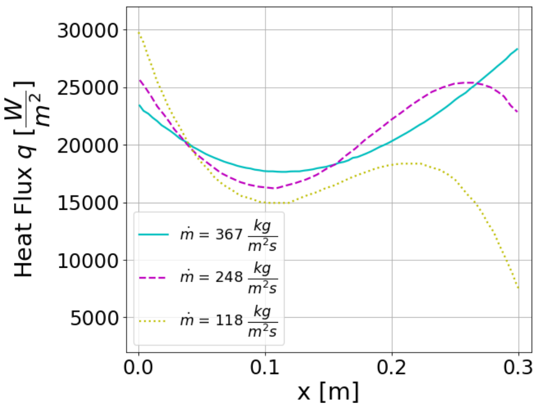
Progress

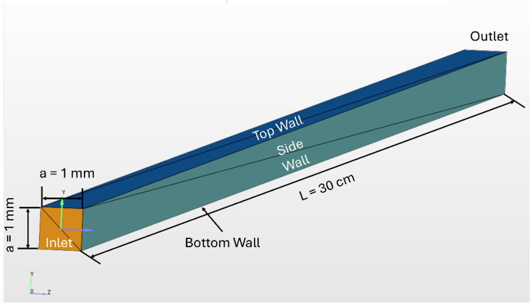
CFD Setup for Microchannel Condensers

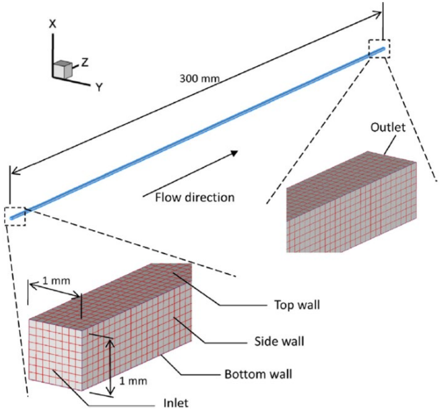
- Multiphase simulations were performed with CONVERGE[1] to model a single microchannel condenser
  - ➢ CFD setup was validated with experiments performed for investigating condensation of FC-72 along parallel square micro-channels[2]
  - ➢ Compressible flow for gas phase and incompressible flow for liquid phase
  - ➢ Volume-of-fluid (VOF) with high-resolution interface capturing (HRIC)[3,4]
  - ➢ Lee condensation model
- Computational cost:
  - ➢ Coarse case: ~2M cells & ~6k CPU hours for 0.3s of flow time
  - ➢ Fine case: ~5M cells & 26k CPU hours for 0.3s of flow time



10 of 1x1 mm² Channels Separated by 1 mm Wide Fins





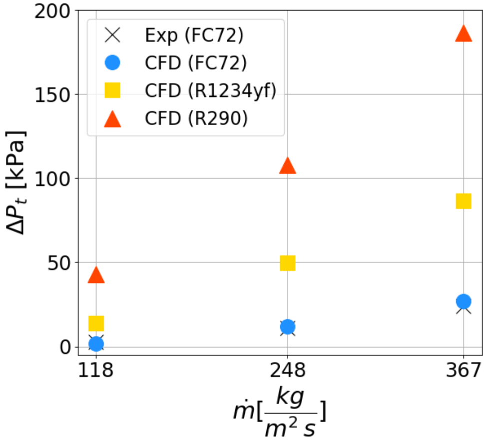


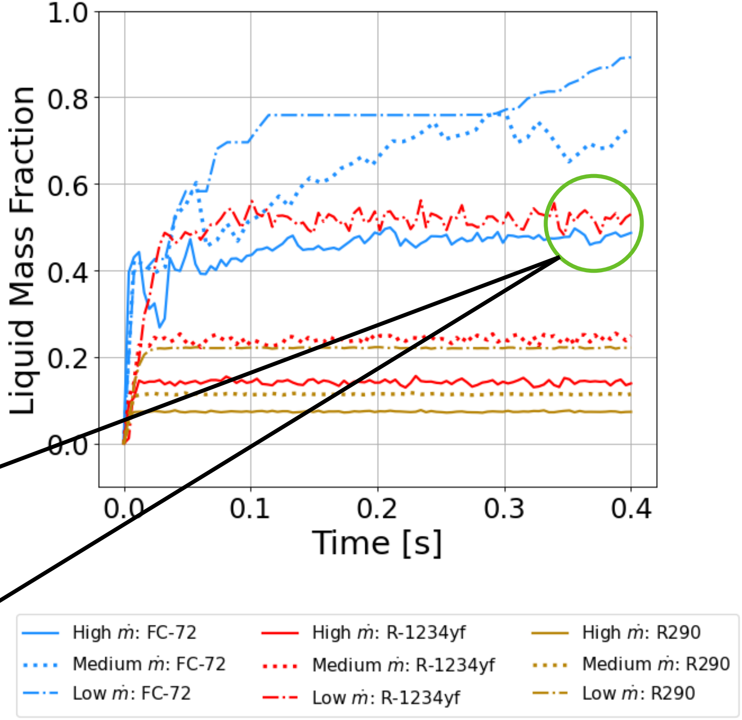
[1]Richards, K., Senecal, P. K., & Pomraning, E. (2023). CONVERGE 3.1 Manual. *Convergent Science Inc., Madison, WI*.
[2]Keniar, K., and Garimella, S. "Experimental investigation of refrigerant condensation in circular and square micro-and mini-channels." *International Journal of Heat and Mass Transfer* 176 (2021): 121383.
[3]Yue, Z., Battistoni, M., & Som, S. (2020). Spray characterization for engine combustion network Spray G injector using high-fidelity simulation with detailed injector geometry. *International Journal of Engine Research*, *21*(1), 226-238.
[4]Magnotti, G. M., Sforzo, B. A., & Powell, C. F. (2022, June). A Computational Investigation of Wall-Film Formation by an Impinging Liquid Jet in Crossflow. In *Turbo Expo: Power for Land, Sea, and Air* (Vol. 85994, p. V03AT04A030). American Society of Mechanical Engineers.

Progress

Microchannel Condensers: Low GWP Refrigerants

Physical Properties	FC-72	R-1234yf	R290
Boiling Point (@ 1 atm) [℃]	56	-29.4	-42.1
GWP [-]	9,300	< 1	3
Critical Temperature [℃]	176	94.7	96.81
Critical Pressure [bar]	18.3	33.82	42.01





High $\dot{m}$, FC-72

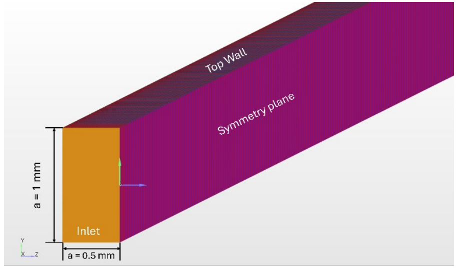
Low $\dot{m}$, R-1234yf

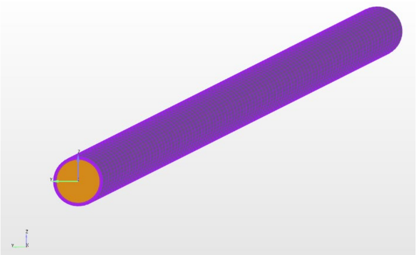
To get similar performance from low GWP refrigerants, need to match inlet operating conditions & boundary conditions

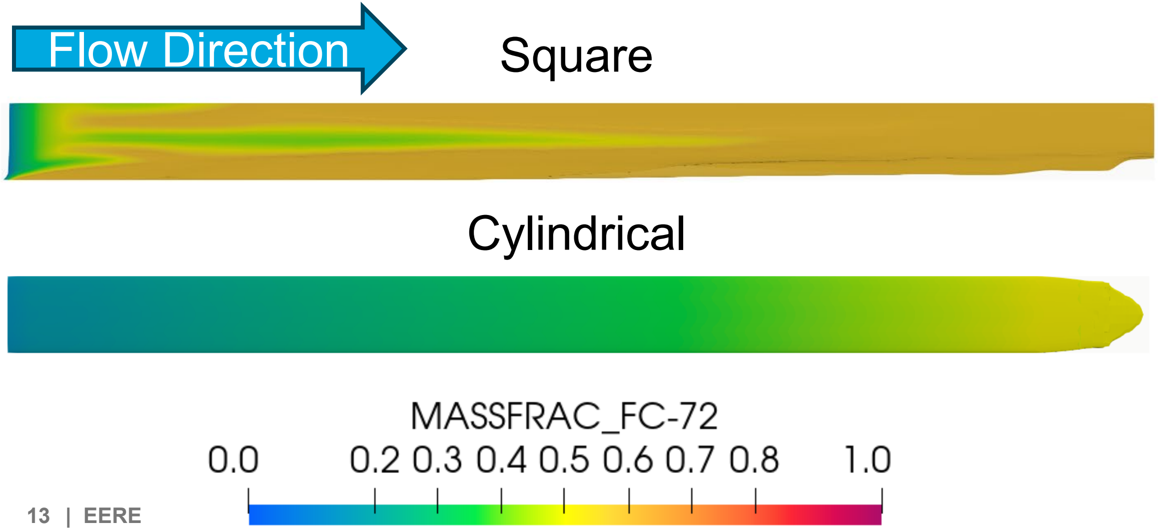
Progress

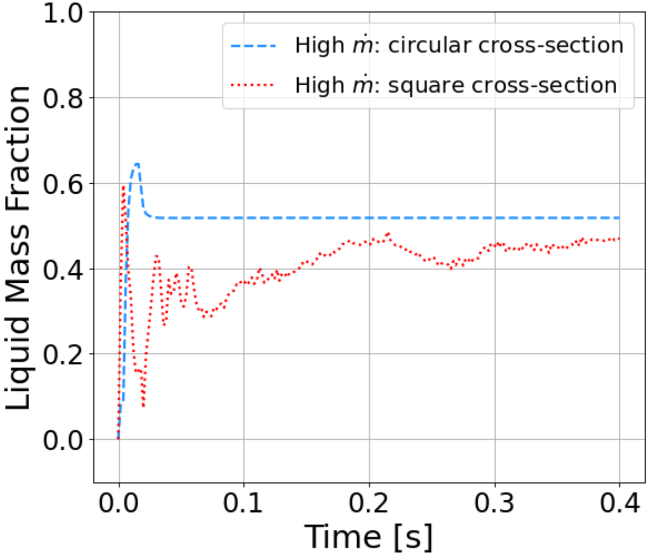
Microchannel Condensers: Cross-Sectional Geometry Effect

- Investigated sensitivity to cross-sectional area for similar operating conditions
- Improved performance found for similar operating conditions with a circular cross-section



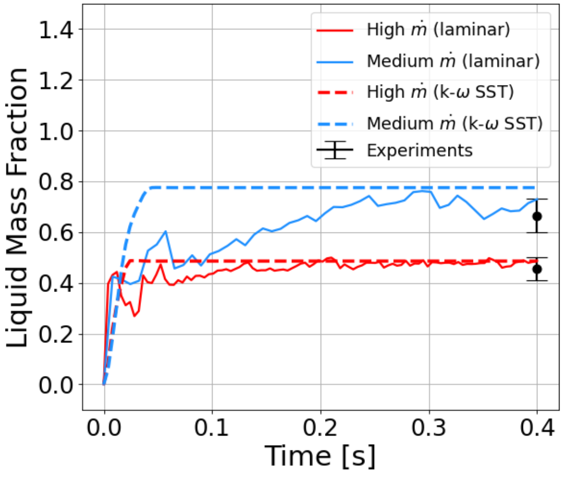


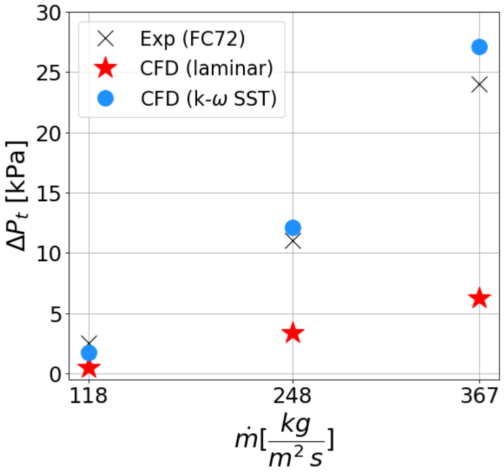


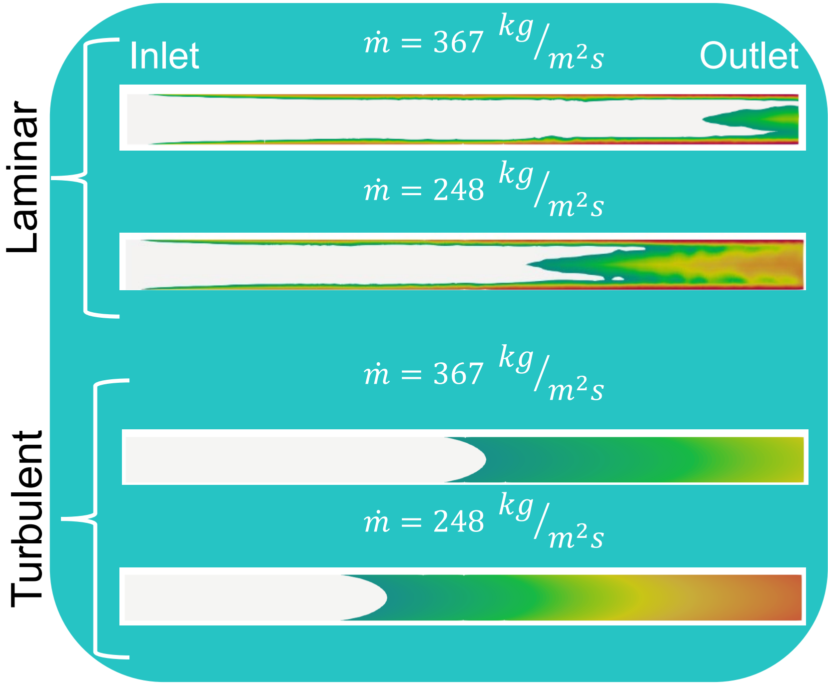


Progress

Microchannel Condensers: Effect of Turbulence Model





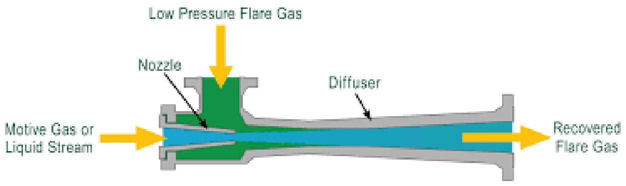


While laminar simulations can capture trends for end state conditions, cannot capture pressure drop, phase change distribution without turbulence modeling

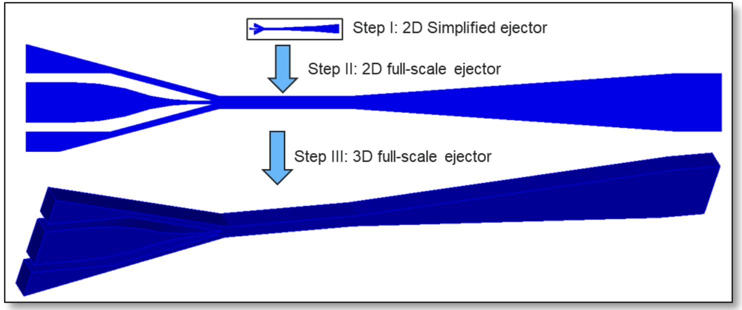
Approach

Modeling Ejector Heat Pumps

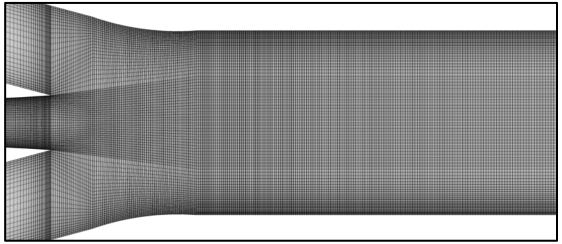
- Ejector heat pumps – promising potential to replace vapor compression cycle for heating/cooling applications:
  - Simple design
  - Lack of moving parts -> reduced maintenance
  - Can operate with low-GWP refrigerants (eg: supercritical CO2)
- There is a lack of accurate CFD or reduced order models for ejectors.
- In the current work, Nek5000[2,3] is used to perform fully-resolved (min. grid size ~5 microns) ejector simulations to develop more accurate reduced order models.



Schematic of a conventional ejector[1]



Computational domain for the ejector simulations

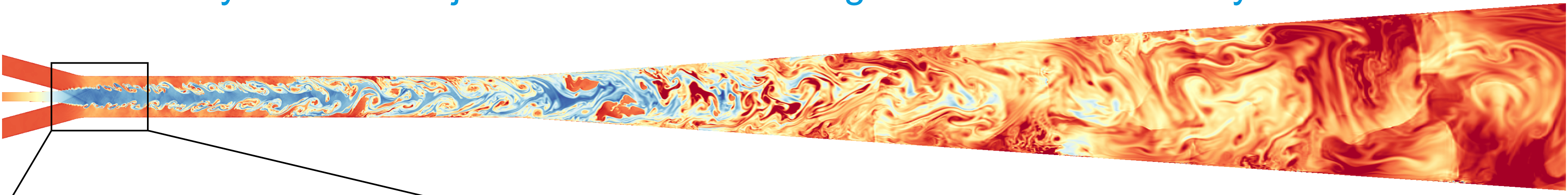


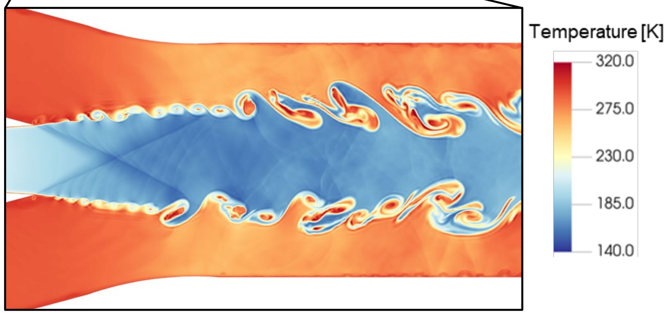
2D plane of the mesh used for the ejector simulations.

[1] https://www.transvac.co.uk/how-an-ejector-works/
[2] Jarrah, I., Pal, P., Ameen, M., & Joly, M. M. (2024). Wall-Resolved LES Study of Shaped-Hole Film Cooling Flow for Varying In-Hole Surface Roughness. In *AIAA AVIATION FORUM AND ASCEND 2024* (p. 4262).
[3] Wu, S., Dasgupta, D., Ameen, M., & Patel, S. (2023). High-Fidelity Simulations of Gas Turbine Combustor using Spectral Element Method. In *AIAA SCITECH 2023 Forum* (p. 1641).

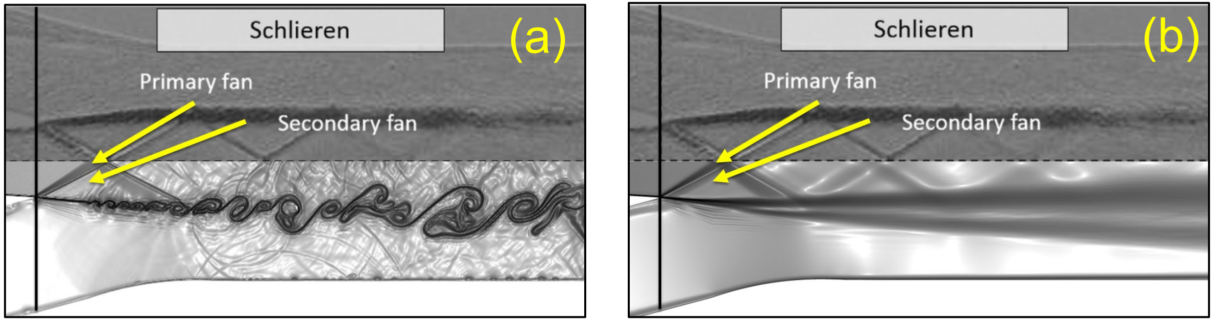
Progress

Fully-Resolved Ejector Simulations using Nek5000: Preliminary Results





Fully resolved simulations using Nek5000



Flow structure at the exit of the primary nozzle. Comparison between Schlieren imagery (experimental) by Croquer et al.[1], and the Nek5000 pseudo-Schlieren $||\nabla\rho||$ (a) Instantaneous (b) Time-averaged.

- Nek5000 simulations capture the shock structures and turbulent flowfield accurately
- Next Step: Use Nek5000 dataset to develop accurate reduced order models

[1] Croquer, Sergio, et al. "Large Eddy Simulation of a supersonic air ejector." Applied Thermal Engineering 209 (2022): 118177.

Progress

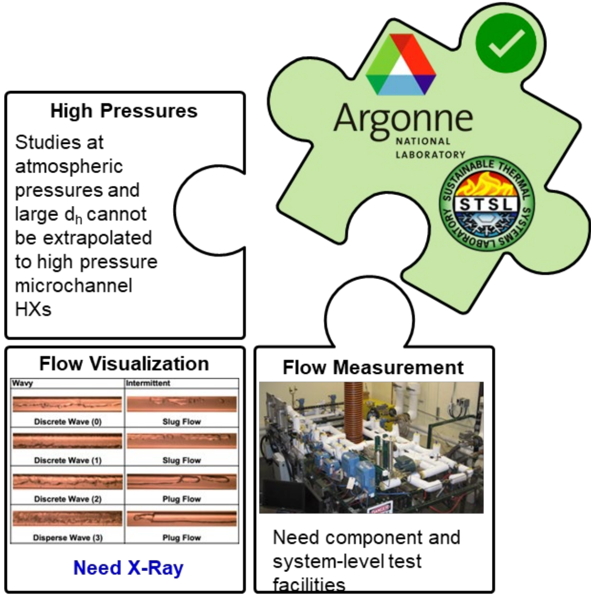
Distributors for evaporators/condensers

Challenge

- Building sector contributes to ~**35% of greenhouse gas emissions**[1]
- Electrification using heat pumps can enable decarbonization
- **Minimizing maldistribution** in two-phase heat exchangers can improve heat pump performance significantly

Approach and Impact

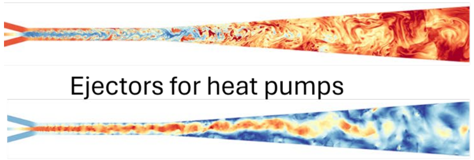
- Develop two-phase distributors to maximize HX performance through even flow vapor quality distribution across channels
- Use fundamental insights from:
  - X-ray flow visualization with high spatial and temporal resolution
  - CFD
  - System-level performance improvement validation
- Potential reduction of total annual US greenhouse gas emissions by 6.5% (412 Million Metric Tons of CO2 equivalent) from the building sector alone
- Heat duty, COP improvement of **up to 50%**[1]

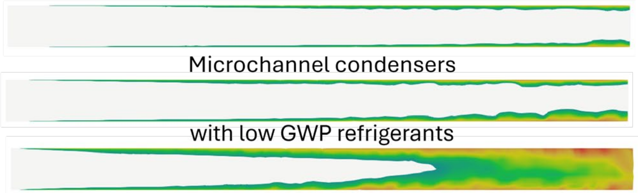


[1] D Forinash. Novel Air-Coupled Heat Exchangers for Waste Heat-Driven Absorption Heat Pumps. 2015

Future Work

- Deliverables:
  - Key findings on the sensitivity of geometric parameters on device performance for conventional and low-GWP refrigerants[1]
  - Data from high-fidelity CFD simulations will be used to developed improved reduced-order models for heat pump design
- Impact (long-term):
  - Accelerate the heat pump design cycle (time-to-market)
  - Increased COP of heat pump due to optimized component designs





[1]Asztalos, Katherine, Muhsin Ameen, Ameya Waikar, and David Rowinski. “Evaluation of Flow, Heat Transfer, and Phase Change Characteristics in Microchannel Condensers using Computational Fluid Dynamic (CFD) Simulations.” Abstract of paper presented at the 2024 Herrick Conferences in Compressor Engineering, Refrigeration and Air Conditioning, and High-Performance Buildings, West Lafayette, IN US, July 15, 2024 – July 18, 2024.

Thank you

Performing Organization(s): Argonne National Laboratory

PI Name and Title:

Muhsin Ameen, Principal Research Scientist

Presenter:

Katherine Asztalos, Research Scientist

PI Email: mameen@anl.gov

WBS #: 3.2.2.63

Reference Slides

Project Execution

	FY2023				FY2024				FY2025			
Planned budget	$200,000				$500,000				TBD			
Spent budget												
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Past Work												
Demonstrate accuracy of modeling microchannel condensers using CFD												
Evaluate effect of microchannel design on performance												
Demonstrate impact of low-GWP refrigerants on condenser performance												
Setup CRADA with Rheem for HPWH optimization (◆ is planned date of milestone)												
Current/Future Work												
CFD modeling of microchannel condensers for heat pump water heater application												
Multi-fidelity simulations to optimize ejector design for heating application												
CFD modeling of refrigerant distribution in evaporator header validated using measurements												

Team FY24

Muhsin Ameen

Principal Research Scientist

Propulsion and Power Department

Katherine Asztalos

Research Scientist

Propulsion and Power Department

Ibrahim Jarrah

Postdoctoral Appointee

Propulsion and Power Department

William Worek

Senior Building Scientist

Energy Systems and Infrastructure Analysis

Sibendu Som

Director

Propulsion and Power Department

Collaborators: Shubham Srivastava (Rheem), Christopher Powell (Argonne National Laboratory), Srinivas Garimella (Georgia Institute of Technology)