Computer-Aided Design and Selection of Optimum Working Fluids and ORC Systems for Power Generation from Low Enthalpy Sources

A. I. Papadopoulos¹, M. Stijepovic², P. Linke², P. Seferlis³, S. Voutetakis¹

¹Chemical Process Engineering Research Institute (CPERI), CERTH, Greece
²Chemical Engineering Department, Texas A&M University at Qatar
³Department of Mechanical Engineering, Aristotle University of Thessaloniki, Greece

INTRO

Conventional Technology
- Databases with heat exchange working fluids
- Evaluation of very limited range of working fluids
- Results feasible but not optimum

Multiple design indices:
- How to combine all of them?
- What should be the performance measure?
- How hard are the constraints?

Computer Aided Molecular Design (CAMD)
- CAMD simulation stage
  - Molecular functional groups e.g. -CH₂-CH₂-OH etc.
  - Candidate working fluid e.g. CH₃OH
- CAMD optimization stage
  - Generation of new performance measure
  - Chemical feasibility constraints
  - Property calculations - Group contribution methods

APPLICATION

Novel Working Fluid and ORC Design Approach

Advisatges at the CAMD stage
- Evaluation of thousands of working fluids
- Computer-aided synthesis of novel molecules
- Consideration of numerous properties

Computer Aided Molecular Design
- Evaluation in ORC systems
- Selection of “optimum” working fluid

Advantages at the ORC design stage
- Evaluation of numerous ORC operating and structural options
- Simultaneous consideration of working fluid candidates
- Gradual increase of ORC modeling details

Power Generation from Low-Enthalpy Geothermal Fields

CAMD fluid design
- Designed commercial fluids
- Designed novel fluids

Commonly used industrial fluids

Economic fluid ORC design performance

CAMD fluid design

Economic fluid ORC design performance

Power and heat cogeneration from varying geothermal fields

Greenhouse power heating cogeneration

Conclusions
- Holistic method for the integrated working fluid and ORC design
- Employs optimization-based CAMD
- Identifies commercially available and novel working fluid options
- Enables simultaneous economic, operating, and safety working fluid and ORC process evaluation

Acknowledgements
This work was partially funded by the John S. Latsis Public Benefit Foundation

Relevant publications