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

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INTRO

Conventional Technology

Databases with heat exchange working fluids

- *Evaluation of very limited range of working fluids*
- *Empirical selection*
- *Results feasible but not optimum*

Evaluation in ORC systems

No ORC design feedback

Selection of "optimum" working fluid

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. $-CH_2-$, OH, $-CH_3$ -COOH etc.

Chemical feasibility constraints

Candidate working fluid
e.g. CH_3-OH

Property calculation- Group contribution methods

CAMD optimization stage

Evaluation of performance measure

Generation of new structure
e.g. CH_3-CH_2-OH

METHODOLOGY

Novel Working Fluid and ORC Design Approach

Computer Aided Molecular Design

Evaluation based on molecular properties

Set of Optimal Working Fluids

Simulation using ORC Models

ORC Process Design Optimization

Evaluation based on ORC economic properties

Optimum ORC and Working Fluid System

Evaluation based on ORC operating properties

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

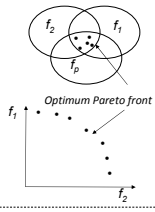
Advantages at the ORC design stage
- *Evaluation of numerous ORC operating and structural options*
- *Simultaneous consideration of working fluid candidates*
- *Gradual increase of ORC modeling details*

Molecular properties	Operating properties
1.Density (ρ)	10. Performance (n)
2.Heat of vaporization (H_v)	11.Max pressure (P_{max})
3. Thermal capacity (C_{pl})	12. Min pressure(P_{min})
4.Viscosity (μ)	13.Mass flowrate (m_f)
5.Thermal conductivity (λ)	14.Critical pressure (P_{max})
6.Melting point (T_m)	
7.Critical temperature (T_c)	
Environmental properties	**Safety properties**
8.Ozone depletion potential (*ODP*))	15.Toxicity (*C*)
9. Global warming potential (*GWP*)	16. Flammability (*F*)

Multi-objective optimization → Set of optimum working fluids

Optimize $f_1, f_2, \ldots, f_p$

Design goals:
Maximize ρ, H_v, λ
Minimize C_{pl}, μ, *ODP*, *GWP*, *C*, *F*
Constraints:
$T_m < T_{min,oper}$
$T_c > T_{max,oper}$



Operating evaluation of working fluids → Economic working fluid evaluation-ORC design

Goals:
Maximize n
Minimize P_{max}, P_{min}, m_f
Constraints $P_{min} > P_{atm}$, $P_c > P_{max,oper}$

Unified performance index

$$I^*_{i,j,l} = \sum_{k=1}^{N} a_{i,j,k,l} \cdot x^*_{i,j,k,l}$$

Minimize

$$I_{i,j,l} = I^*_{i,j,l} + pen_{i,j,l}$$

Goals:
Maximize $f = \frac{10 x R_{gross}}{C_{CAP}}$
Decision parameters:
Vaporizer, condenser type, areas, Turbine type, size tec.

APPLICATION

Power Generation from Low-Enthalpy Geothermal Fields

CAMD fluid design

Designed commercial fluids

ID	Molecular type and name	CAS Registry number	η (%)	P_{max} (atm)	P_{min} (atm)	m (kg/hr)	$I_{2D,SQ,l}$	F	C
	Hydrocarbons								
1	Butane	106-97-8	7.51	9.85	3.23	13069	0.016	0.564	1.94
2	2-Methyl-1,3-butadiene	78-79-5	8.02	3.77	1.08	12840	-1.702	0.589	2.49
3	2-Methyl-1-butene	563-46-2	7.88	4.14	1.15	12869	-1.620	0.594	2.83
4	1,4-Pentadiene	591-93-5	7.94	4.62	1.47	14230	-1.297	0.622	1.54
5	1,3,5-Hexatriene	821-07-8	8.18	1.28	0.28	12152	2.744	0.665	1.91
6	1,3-Butadiene	106-99-0	7.64	11.29	3.72	12699	0.377	0.592	1.25
	HFCs								
7	1,1,1,3,3,3-Hexafluoro-2,3,3-Trifluoro-propene	690-39-1	6.61	18.00	6.07	37611	4.608	MA[c]	2.84
8		677-21-4	6.82	21.22	7.54	27580	4.682	0.409	2.19
	Fluorinated ethers								
9	Methoxy methyl-fluoride	460-22-0	8.12	6.27	1.75	12683	-1.104	0.584	0.97
10	Methyl-trifluoromethyl-ether	421-14-7	7.27	16.98	5.61	24892	3.074	0.513	1.54
11	1,1,1-Trifluoro-methoxy-ethane	460-43-5	7.88	4.24	1.09	19695	-0.977	0.528	1.84
12	2,2,2-Trifluoro-ethyl-ethyl-ether	461-24-5	7.85	3.05	0.72	20098	2.905	0.538	2.13
	Ethers								
13	Methoxy-ethene	107-25-5	7.88	9.38	2.82	12469	-0.265	0.721	0.89
14	Methoxy-ethane	540-67-0	7.78	8.82	2.68	12620	-0.388	0.595	1.24
15	Dimethyl-ether	115-10-6	7.32	22.19	7.72	12828	3.486	0.567	0.95
16	Dimethoxy-	109-87-5	8.20	3.23	0.79	13030	2.114	0.601	0.83
17	2-Methoxy-1-	116-11-0	8.19	2.29	0.55	11845	2.342	0.642	2.13
18	Methyl-propyl-ether	557-17-5	8.02	3.44	0.87	12585	1.957	0.600	1.54
19	3-Methoxy-1-	627-40-7	8.19	2.63	0.63	11983	2.239	0.642	1.19
20	3-Ethenyloxy-1-propene	3917-15-5	8.19	1.72	0.38	12875	2.690	0.664	1.13
	Amines								
21	N-Methyl-methanamine	124-40-3	7.94	9.98	2.82	9246	-0.487	0.559	1.24
22	N-Methyl-	624-78-2	8.29	2.31	0.51	9300	2.185	0.578	1.54
23	N,N-Dimethylallyl amine	2155-94-4	8.17	1.02	0.20	11928	2.845	MA[b]	1.57
	Formates								
24	Methyl-formate	107-31-3	8.33	4.57	1.14	10806	-1.759	0.558	1.60
	Aldehydes								
25	Trifluoro-	75-90-1	7.92	8.65	2.37	19206	0.095	0.443	2.60
26	Acetaldehyde	75-07-0	8.28	5.96	1.54	8370	-1.638	0.667	2.01
	Alcohols								
27	Methanol	67-56-1	8.60	1.84	0.27	4204	2.097	0.591	1.02

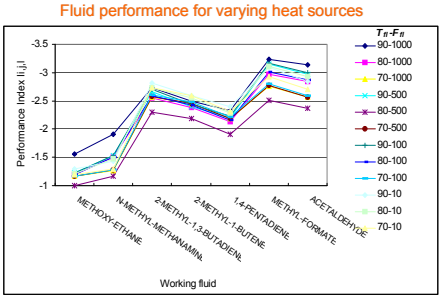
Designed novel fluids

ID	Molecular type and name	η (%)	P_{max} (atm)	P_{min} (atm)	m (kg/hr)	$I_{2D,SQ,l}$	F	C
	Fluorinated Amines and Ethers-Amines							
28	CF_3-CH_2-NH_2	8.05	4.65	1.12	16685	-1.194	0.447	1.75
29	CF_3-CH(CF_3)-NH_2	7.97	1.78	0.34	22562	3.695	0.406	3.06
30	CH_2-NH-CF_3	8.04	4.71	1.17	17178	-1.119	0.477	1.84
31	CH_3-OCH$_2$-NH_2	8.42	1.31	0.24	8595	2.498	0.584	0.75
	Fluorinated Ethers							
32	FCH_2-O-CH_2-OCF_3	8.15	1.11	0.20	19325	3.574	0.524	1.44
33	FCH_2-O-CF_3	7.82	9.59	2.82	24190	0.977	0.406	1.56
34	CH_3-CH-CH_2-O-CF_3	7.82	3.78	0.94	20880	2.643	0.559	1.78

Commonly used industrial fluids

ID	Molecular type and name	η (%)	P_{max} (atm)	P_{min} (atm)	m (kg/hr)	$I_{2D,SQ,l}$
	Industrial fluids					
35	1,1,1,2-Tetrafluoroethane	6.58	25.48	8.75	29464	5.934
36	Water	4.78	0.43	0.05	26672	4.466
37	1,1-Difluoroethane	7.11	22.99	7.85	18716	4.209
38	1,1,1,2,2-Pentafluoropropane	6.59	17.70	6.06	34417	4.257
39	1,1,1,2,3,3-Hexafluoropropane	7.40	9.88	2.83	30025	1.479
40	1,1,1,2,3,3,3-Heptafluoropropane	6.36	17.94	6.01	42377	5.030
42	Cyclopropane	7.24	24.85	9.28	13089	4.495
42	Trifluorodichloromethane	7.26	17.69	6.35	59648	6.487
43	Perfluoro-n-pentane	6.72	4.51	1.22	45679	1.582
44	2-Methyl-Butane	7.70	4.52	1.30	13356	-1.460
45	2,2-Dimethyl-Propane	7.41	7.17	2.29	15002	-0.543
46	N-Hexane	7.96	1.40	0.30	12546	2.760
47	Bis-Difluoromethly-Ether	7.62	10.28	2.91	23526	0.946
48	2-Difluoromethoxy-1,1,1-Trifluoro	7.69	5.01	1.25	25034	-0.298
49	Ethanol	8.52	1.12	0.14	5528	2.362

Fluid performance for varying heat sources

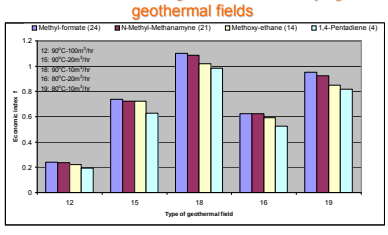


ORC process design

Economic fluid-ORC design performance

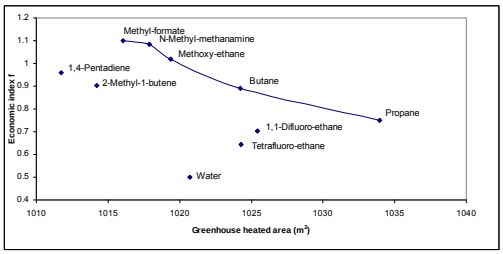
ID	Molecular type and name	Vaporizer Area (m²)	Vaporizer Cost ($)	Condenser Area (m²)	Condenser Cost ($)	f
24	Methyl formate	125.8	28940	45.5	18920	1.1
21	N-Methyl-methanamine	108.7	26020	45.5	19390	1.08
(M1)	Methanol	87.1	28040	76.6	23410	1.05
14	Methoxy-ethane	120.7	26970	40.9	19480	1.02
4	1,4-Pentadiene	147	31510	52	19140	0.96
3	2-Methyl-1-butene	163.5	33210	65.7	21220	0.90
1	Butane	146.8	32350	45.5	18320	0.89
M5	Propane	36.1	19060	47.7	21810	0.75
M3	1,1-Difluoro-ethane	146.1	35100	58.3	22370	0.70
M4	Tetrafluoroethane	198.2	40320	50.5	20990	0.64
M6	Water	78.3	21690	604.1	85990	0.49

Power and heat cogeneration from varying geothermal fields



Greenhouse power-heating cogeneration

Economic-heating performance trade-offs



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, environmental and safety working fluid and ORC process evaluation

Acknowledgements

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Associated publications

- A.I. Papadopoulos, M. Stijepovic, P. Linke, *Applied Thermal Engineering* 30 (2010), 760-769
- A.I. Papadopoulos, M. Stijepovic, P. Linke, P. Seferlis, S. Voutetakis, *Chemical Engineering Transactions* 25 (2011) 61-66