

**RAY W. HERRICK**  
**LABORATORIES**

A Moving Boundary Modeling Approach for  
Heat Exchangers with Binary Mixtures

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# Outline

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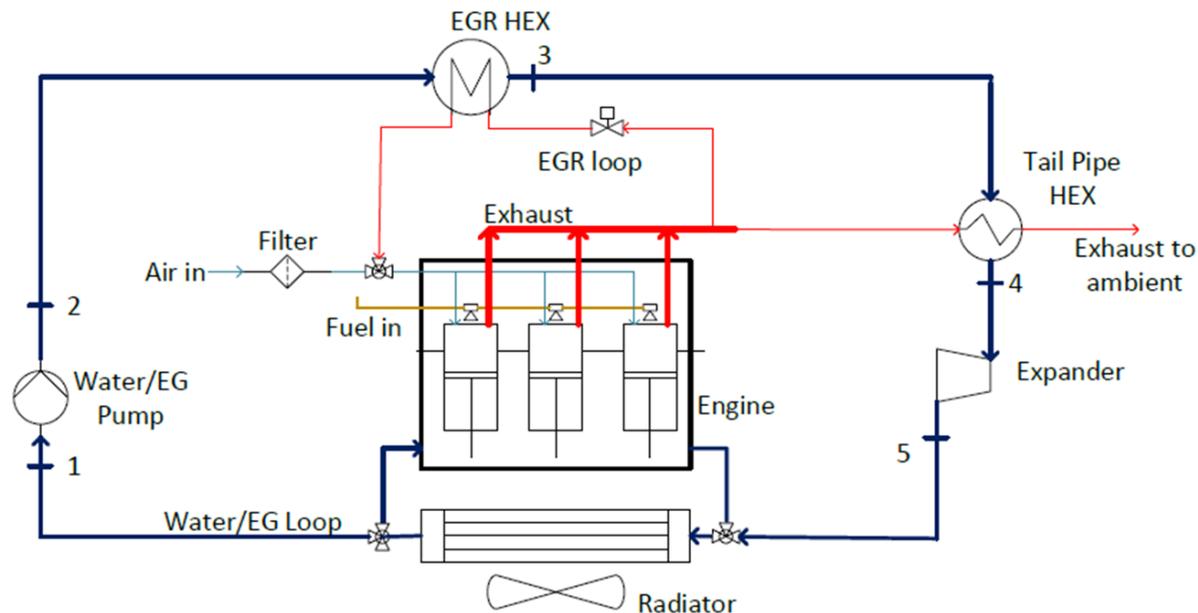
- ❑ Introduction
- ❑ Research Objectives
- ❑ Motivating Example
- ❑ Modeling Approach
- ❑ Results
- ❑ Conclusions and Future Work

# Introduction (1/2)

- Heavy Duty Diesel Engines (HDDEs) reject a considerable amount of energy to the ambient
- In order to meet the U.S. Department of Energy (DOE) break thermal efficiency (BTE) goals, WHR by means of ORCs has been identified by U.S. engine manufacturers as viable solution
- Research on ORC systems applied to passenger and commercial vehicles has flourished in recent years
  - ❑ Subcritical and transcritical cycles (e.g., Amicabile et al. 2015)
  - ❑ Cascade cycles (e.g., Chen et al. 2017)
- Cost, complexity, environmental concerns and safety considerations are major issues that hold back OEMs from adopting ORCs in vehicles

# Introduction (2/2)

- An affordable Rankine cycle (ARC) system is proposed in order to obtain real benefits of WHR on the road and reduce the costs by 50% with a targeted payback period of 1.4 to 2 years
- A novel ORC architecture proposed within the ARC project is based on using the engine coolant, i.e., **mixture of water/EG**, as the working fluid.



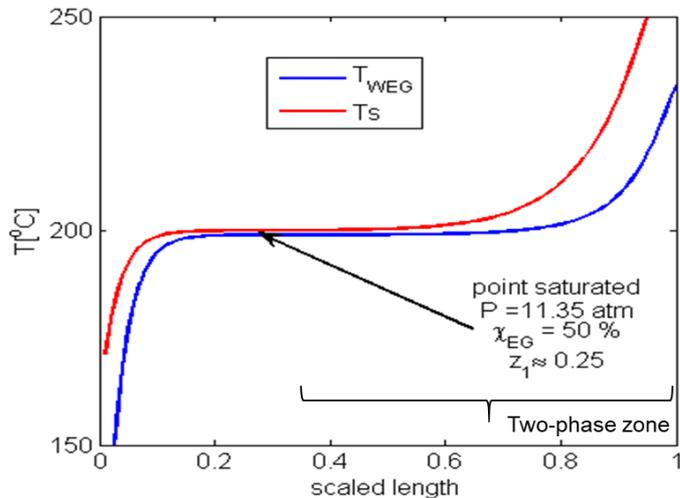
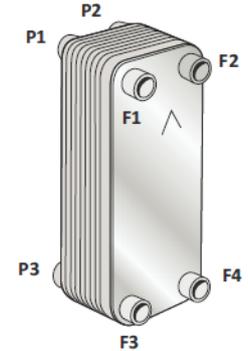
# Research Objectives

- A thermodynamic feasibility study has been performed and reported in a companion paper<sup>[1]</sup>.
- As waste heat recovery from an engine is a highly transient process, dynamic modeling is necessary to design the system
- This paper describes the initial dynamic modeling efforts for the ORC system, with focus on heat exchangers, using the mixture W/EG
- MB formulation: essential to assume a spatial enthalpy profile, typically linear, in lumping a number of control volumes
- Therefore, the MB can possibly result in a poor prediction when the approximation fails:
  - This paper starts from a motivating example for this case
  - Introduces a more reliable MB formulation

<sup>[1]</sup>Ziviani et al., "Feasibility Study of ICE Bottoming ORC with Water/EG Mixture as Working Fluid" Energy Procedia 129(2017), 762-769

# Motivating example (1/2)

- A detailed heat exchanger model was developed using FVM
- The static HX model working with R245fa and steam was validated with experiments for more than 70 operating conditions
- After the validation, the working fluid has been replaced to W/EG (50/50) on the static FVM model



- An example temperature profiles (steady state)
- 100 nodes for FVM
- REFPROP for properties
- Note  $T_{WEG}$  in TP zone is away from a linear profile.

Temperature profiles at evaporator with W/EG (FVM[100])

Boundary condition	$P$ [atm]	$\dot{m}$ [kg/s]	$h_i$ [kJ/kg]	$\dot{m}_s$ [kg/s]	$T_{s,i}$ [°C]
Values	11.35	0.10	-23	0.62	280

# Motivating example (2/2)

- MB under the same boundary conditions was implemented: a static MB model was retrieved by eliminating time-derivative terms of a transient MB model [2]
- 12.54% difference in heat transfer rate.
- Significant difference in the length for the subcooled liquid zone: MB predicts 4% while FVM predicts 25%.
- The poor estimation on the length could significantly influence on behaviors of a dynamic MB cycle model

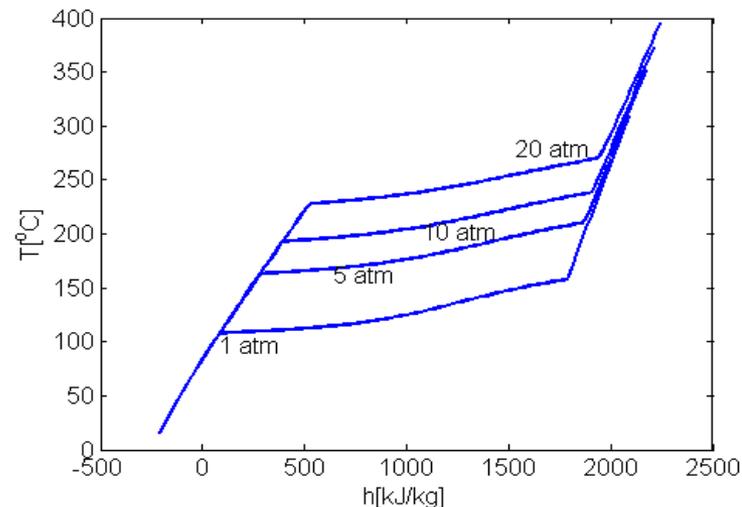
Result comparisons between FVM and MB

	$h_e$ [kJ/kg]	$z_1$ [-]	$\bar{T}_{s,1}$ [°C]	$\bar{T}_{s,2}$ [°C]	$\dot{Q}$ [kW]
FVM	1649.2	0.25	194.23	209.74	167.22
MB	1439.5	0.04	183.97	212.78	146.25

[2] Bendapudi, S., Braun, J. E., & Groll, E. A. (2008). A comparison of moving-boundary and finite-volume formulations for transients in centrifugal chillers. *International Journal of Refrigeration*, 31(8), 1437-1452.

# Modeling Approach (1/3)

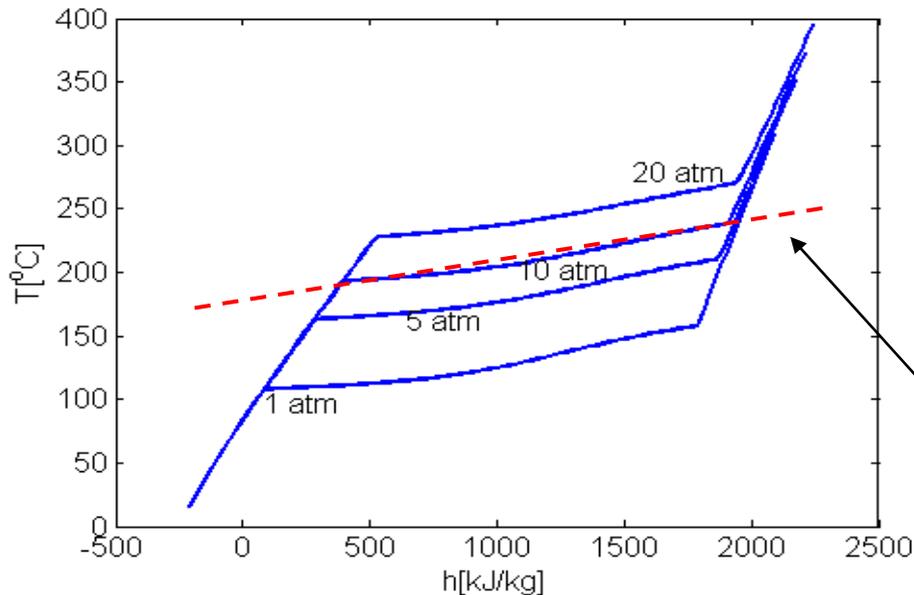
- One main assumption for MB formulation (standard assumptions in dynamic MB modeling): spatial enthalpy distribution of the working fluid is linear.
- Linear spatial distribution enthalpy for each zone implies a linear spatial distribution of temperature for the zone
- However, temperature profile in the TP zone was not linear → the enthalpy distribution is not linear in our case due to temperature glide.



T-h diagram for water/ethylene glycol mixture (50/50) [REFPROP]

# Modeling Approach (2/3)

- Our approach to handle this problem is to include appropriate spatial temperature profiles for both streams for each zone
- Assumption: linear relationship between changes of temperature and enthalpy for any phase zones



- It allows to define isobaric specific heat capacity
- Example for TP zone

$$c_{p,2} := \frac{\partial h}{\partial T} \approx \frac{h_g(P, \chi_{EG}) - h_f(P, \chi_{EG})}{T_g(P, \chi_{EG}) - T_f(P, \chi_{EG})}$$

T-h diagram for water/ethylene glycol mixture (50/50)

# Modeling Approach (3/3)

- With this assumption, the heat transfer problem for a binary mixture can be converted to a standard heat exchanger problem, i.e. for each phase,

$$\frac{dT_s}{dx} = \frac{NTU_s}{L} (T_s - T_p)$$
$$\frac{dT_p}{dx} = \frac{NTU_p}{L} (T_s - T_p)$$

- This allows to use the  $\epsilon$ -NTU or LMTD like approach
- Note that those approaches uses analytic temperature profiles for both fluids
- Those approaches were reformulated to be integrated to MB formulation

# Results (1/2)

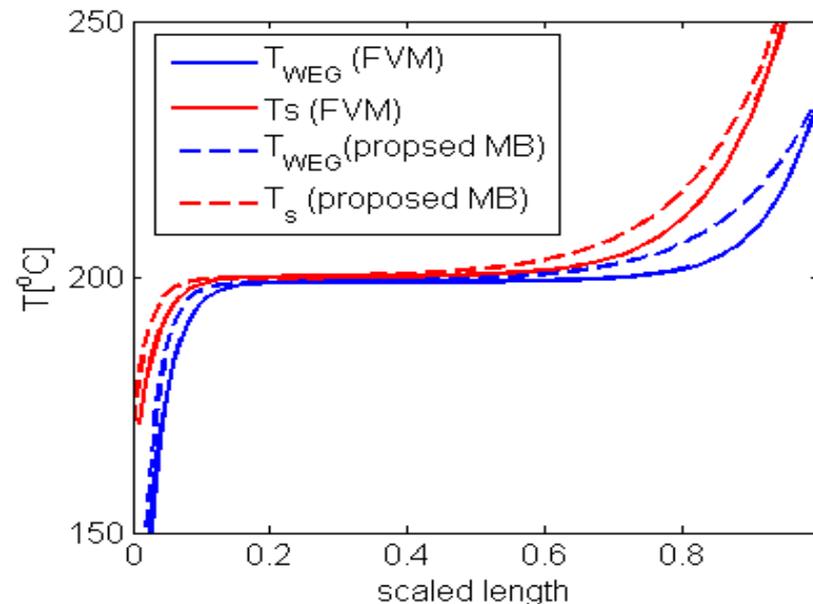
- The same problem was solved
- REFPROP is used to calculate specific heat capacities in liquid and TP zones
- The presented MB makes substantially better agreements on the exit enthalpy, subcooling length and mean temperatures of secondary flow compared with the conventional MB

Result comparisons between each approach

	$h_e$ [kJ/kg]	$z_1$ [-]	$\bar{T}_{s,1}$ [°C]	$\bar{T}_{s,1}$ [°C]	$\dot{Q}$ [kW]
FVM	1649.2	0.25	194.23	209.74	167.22
Conventional MB	1439.5	0.04	183.97	212.78	146.25
Proposed MB	1648.9	0.28	196.33	212.73	167.19

# Results (2/2)

- Real benefit is in the capability to retrieve spatial distributions of temperature, enthalpy and density from the calculated mean and inlet temperatures. → better charge estimation
- This is possible because of the analytic temperature profiles
- The proposed MB is 2.74 times slower than that of the conventional MB, but is 4.95 times faster than the 20-node FVM



Comparison of temperature profiles between FVM and proposed MB

# Conclusions and Future Work

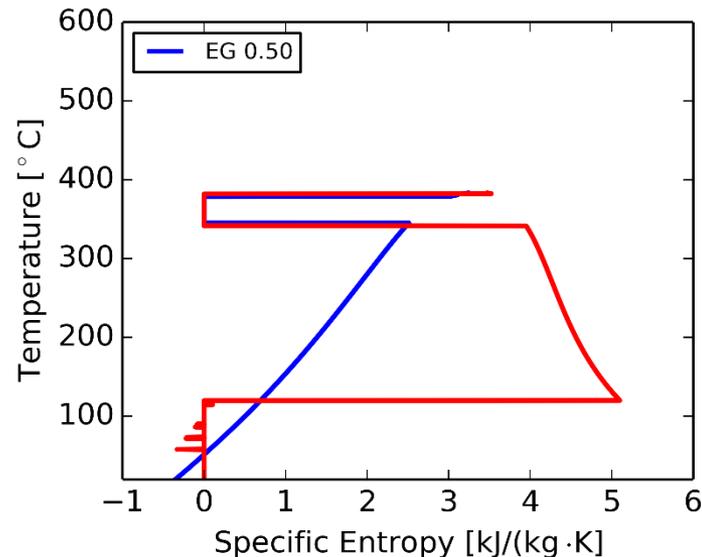
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- ❑ MB assuming a linear spatial distribution of enthalpy could result in a considerable error, due to the temperature glide of a binary mixture
- ❑ A more reliable MB method is presented by incorporating analytic steady temperature profiles for a binary mixture.
- ❑ The proposed method shows substantially better agreements with FVM.
- ❑ Spatial distributions of thermodynamic states can be retrieved using available states, and hence it will significantly improve charge estimation within the MB framework.
- ❑ The approach will be applied to a dynamic MB model and its performance will be tested with transient data for an ORC test-rig.

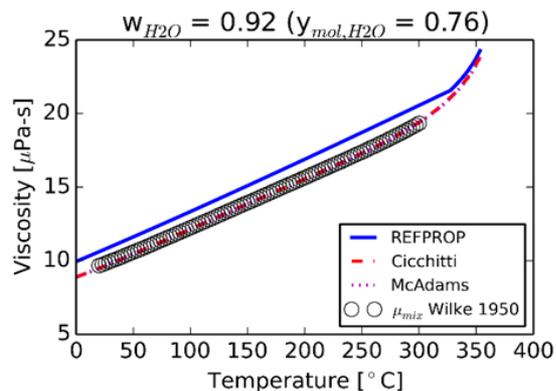
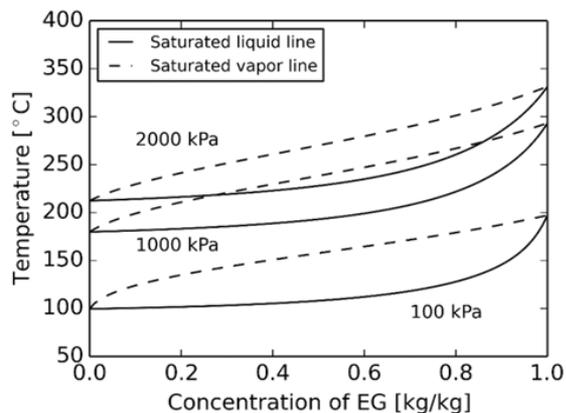
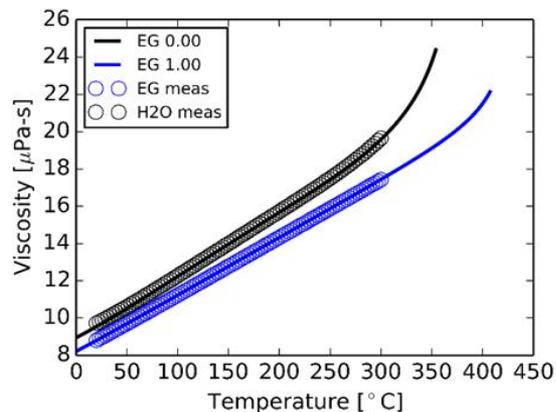
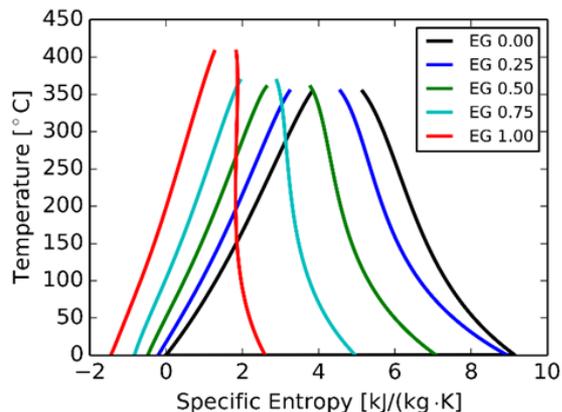
Thank you  
&  
Questions?

# Appendix. Thermophysical Properties of Water/EG Mixture (1/2)

- ❑ The working fluid is a binary mixture of water and ethylene glycol.
- ❑ Few studies are available about thermodynamic and transport properties, e.g., Teja et al. 2003 and Dai et al. 2011.
- ❑ As the mixture phase-change is an important aspect, VLE conditions need to be obtained to understand the effect of concentration shifting.
- ❑ Original Water/EG mixture REFPROP file had issues:



# Appendix. Thermophysical Properties of Water/EG Mixture (2/2)



□ Updated Water/EG mixture available within REFPROP 10.0 release