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Thermodynamic Cycle Analysis Program (TCAP)

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Thermodynamic Cycle Analysis Program (TCAP)

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Abstract

This report describes the Thermodynamic Cycle Analysis Program (TCAP) software developed in support of the Collaborative Advanced Gas Turbine (CAGT) research project. The goal of the CAGT project was to evaluate different configurations of gas turbine-based power generation cycles. TCAP software enables the user to graphically construct power cycles that incorporate a variety of components such as compressors, turbines, heat exchangers, and reactors. The user also specifies the input condition of the working fluid and the parameters associated with each component. TCAP then calculates the composition and thermodynamic properties of the working fluid at every point in the cycle. From this data, TCAP calculates the overall thermodynamic efficiency of the cycle and emission levels of specific chemicals. Thermodynamic and chemical kinetic data are based on the Chemkin family of application codes and libraries.

Acknowledgments

The author thanks A. E. Lutz of the Mechanics and Simulation of Manufacturing Processes Department for his contributions in interfacing the TCAP software with Chemkin applications and libraries, and P. K. Falcone of the Systems Studies Department for her leadership in Sandia's support of the CAGT Project.

Thermodynamic Cycle Analysis Program (TCAP)

Introduction

The Collaborative Advanced Gas Turbine (CAGT) project was launched in 1992 by the California Energy Commission and several power utilities, including the Pacific Gas and Electric Company. The goal of the project was to evaluate several proposed configurations for gas turbine-based power generation cycles. Two of the key metrics were (1) thermodynamic efficiency and (2) the level of NO_x and SO_x emissions produced. Several commercial tools that calculate thermodynamic efficiencies of power cycles were available. However, these programs were limited to modeling non-reacting fluids or fluids always in a state of chemical equilibrium. They could not predict emission levels produced by chemical reactions in a combustor in the cycle.

We developed the Thermodynamic Cycle Analysis Program (TCAP) to provide the capability of predicting emission levels as well as thermodynamic efficiency. This required the incorporation of chemical *kinetics* modeling as well as equilibrium thermodynamic property modeling.

This report describes the design and functionality of the TCAP software.

Cycle Construction

In TCAP, power cycles are composed of *components* and *connections*. Components represent turbines, compressors, combustors, and other physical parts of the power generation cycle. Each type of component has a variable number of parameters that describe its behavior. For example, a turbine component has three parameters: the number of effective stages, the pressure ratio, and the isentropic efficiency. A complete list of components is given in the Appendix.

A connection links two components together and can be one of three types: fluid, work, or heat. A fluid connection represents the flow of fluid from the outlet of one component to the inlet of the other. A work connection represents the transfer of mechanical work from one component to another (e.g. from a turbine to a compressor). A heat connection represents the transfer of sensible heat from one component to another (e.g. from a combustor to a heater).

Fluid connections represent the working fluid of the cycle. The fluid is characterized by its composition (a list of chemical species and their relative amounts), its flowrate, and its

thermodynamic properties (temperature, pressure, enthalpy, and entropy). Work connections are characterized by the work rate (power) being transferred; heat connections by the heat rate.

TCAP is extremely flexible in its support of cycle configurations: cycles can be composed of any combination of any number of components. There is also no limit to the number of connections in a cycle, although individual components may restrict the number and type of connections that can be linked to it. For example, a turbine must have one inlet fluid stream and one outlet fluid stream, and may have one outgoing work connection. A heater must have one inlet fluid stream and one outlet stream, and may have an incoming heat connection (the incoming heat energy is transferred to the fluid flowing through the heater).

Figure 1. The main window of TCAP's graphical user interface.

Cycles are constructed using TCAP's graphical user interface. The main window comprises two sections: a palette of components and a drawing area (Figure 1). On the palette are icon representations of all of the components that can be modeled. To add a component to the cycle, the user clicks on the appropriate icon, then places it on the drawing area. Clicking on the placed icon brings up another window that displays the parameters associated with the component. In this window, values for each of the parameters may be entered or edited by the user. This is illustrated in Figure 2 for a Turbine.

Figure 2. Editing window for a component.

All three types of connections are created by first specifying the source component, then the destination component for the fluid, work, or energy stream. Once the connection is created, clicking on it brings up a window that displays the associated thermodynamic properties or parameters. As with components, values of the properties or parameters may be entered or edited by the user. This is illustrated in Figure 3 for a fluid connection.

Figure 3. Editing window for a fluid connection.

An example of a completed cycle is shown in Figure 4. This is a very basic cycle configuration in which the working fluid emerges from a fluid source and is compressed,

heated, and expanded through a turbine before it enters a fluid sink. The following properties and parameters have been specified for the cycle:

Fluid state 1:	composition	air (78% N ₂ , 21% O ₂ , 1% Ar)
	temperature	288K
	pressure	1 atmosphere
	mass flowrate	1 kilogram/second
Compressor:	number of stages	1
	pressure ratio per stage	12
	isentropic efficiency	0.87
Fluid state 3:	temperature	1400K
Turbine:	number of stages	1
	isentropic efficiency	0.95
Fluid state 4:	pressure	1 atmosphere

Figure 4. A basic air cycle.

An example of a more complex cycle configuration is shown in Figure 5.

The behavior of a component is defined by equations that relate the properties of the inlet and outlet fluid streams and the energy transfer of the work and heat connections. For example, a turbine's behavior is described in part by the following equations:

$$\dot{m}_{inlet} = \dot{m}_{outlet} \quad \text{Equation (1)}$$

$$P_{inlet} = P_{outlet} \cdot r^n \quad \text{Equation (2)}$$

where $\dot{m}$ is the mass flowrate, p is the fluid pressure, r is the pressure ratio per stage, n is the number of stages, and *inlet* and *outlet* refer to the inlet and outlet fluid streams. Equation (1) is a continuity equation, stating that no fluid is lost or created within the turbine. Equation (2) states the relationship between the inlet and outlet fluid pressures based on turbine parameters. If the inlet flowrate has been specified by the user (or has been previously calculated), then TCAP will calculate the outlet flowrate (and vice-versa). Similarly, if one of the fluid pressures is known, TCAP will calculate the other, provided the turbine parameters have been defined.

Some of the component behaviors involve more complex relationships. An equilibrator component brings a fluid to an equilibrium state. TP-Equilibrators bring the fluid to *chemical* equilibrium at constant temperature and pressure, while TP-Phase Equibrators bring the fluid to a *phase* equilibrium (no chemical reaction) at constant temperature and pressure. All equilibrium calculations are performed with a Chemkin-based implementation of the Stanjan² solver. The PFR component models a plug flow reactor with a specified residence time, while the PSR component models a perfectly stirred reactor, also with a specified residence time. The behavior equations of the PFR and PSR components are based on the Senkin³ code and the PSR⁴ code respectively. Behavior equations for all components are listed in the Appendix.

Once the cycle is constructed and parameters have been specified, TCAP attempts to calculate thermodynamic properties for each fluid state in the cycle. There are two solution modes: direct and iterative.

In the direct solution mode, TCAP searches through the cycle for unspecified properties. When it finds one, TCAP calculates the value of the property if there is enough information to calculate it directly. This will be true if the property is the only unknown variable in an equation of state or behavior equation. The search and calculate procedure is repeated until all fluid states are defined and the solution is complete. The direct solution mode succeeds for many cycle configurations. However, some configurations, especially those with closed loops, cannot be solved in this fashion. In these cases, TCAP attempts the iterative solution mode.

In the iterative solution mode, equations of state and behavior equations are set up as a single system of simultaneous equations, where the unknown variables are the unspecified thermodynamic properties. If the cycle has been properly constructed, the number of equations will be equal to the number of unknown properties, and TCAP will

solve for the properties using an iterative solution algorithm named TJMAR1⁵. This solution mode is computationally more intensive than the direct mode, but is also more powerful.

STATE	MASS FLOW kg/s	MOLAR FLOW mole/s	TEMP deg K	PRESSURE atmos	ENTHALPY kJ/kg	ENTROPY kJ/kg K
1	1.000**	34.519*	298.000**	1.000**	-10.135*	6.824*
2	1.000*	34.519*	622.343*	12.000*	332.583*	6.898*
3	1.000*	34.519*	1400.000**	12.000*	1216.501*	7.812*
4	1.000*	34.519*	825.769*	1.000**	551.890*	7.916*

Efficiency Calculation:
 Net power out () KW: 321.893424
 Efficiency () %: 0.364166

Figure 6. Solution printout for the basic air cycle.

When the cycle solution is complete, TCAP prints out a table of all fluid properties. The printout for the basic cycle of Figure 4 is displayed in Figure 6. The program keeps track of the origin of each of the property values. Those that were specified by the user are marked with a double asterisk (**). Calculated values are marked with a single asterisk (*). Value origins are also identified on the cycle drawing. In Figure 7, the color of each fluid connection corresponds to the origin of the fluid temperature. Green denotes a user specified temperature, yellow denotes a calculated value. If any fluid temperature were still unknown, it would be colored red.

Figure 7. The basic cycle with fluid color-coding based on the origin of the temperature value.

The thermodynamic efficiency is calculated as the net available turbine work divided by the net energy input to the cycle. Energy input includes both sensible heat (which flows

into heaters and reformers) and the latent heat of the working fluid. Emission levels are determined by analyzing fluid streams that flow into sinks, as these represent fluids that flow out of the cycle into the surrounding environment. From the flowrates and compositions of these streams, the emission level can be calculated for any chemical species of interest.

Conclusion

The TCAP software was developed to support the analysis needs of the CAGT project. With TCAP, a user can quickly construct thermodynamic cycles using a graphical user interface. No programming skills are required. TCAP can solve for the thermodynamic states of the fluid throughout the cycle, and from this data the thermodynamic efficiency and emission levels can be determined for the cycle.

The modeling of components in TCAP is done on a fairly simple and generic level. In particular, the components that are used to represent a combustion engine are not nearly as detailed as other models, both commercial⁶ and proprietary, that have been developed for specific makes of engines. These customized models often require dozens of input variables. Although TCAP cannot approach this level of detail, the CAGT Project analysts believed that TCAP would be sufficiently accurate for their comparative study of cycle configurations, and could serve as a common base-line analysis tool.

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Appendix

Component Behavior

Nomenclature used throughout this appendix:

Fluid streams:	T	temperature
	p	pressure
	$\dot{m}$	mass flow rate
	h	specific enthalpy
	x_i	mass fraction of chemical species i
	x	mass composition of fluid (includes specification of all x_i)
	s	specific entropy
	v	specific volume
Work:	$\dot{W}$	work per unit time (power)
Heat transfer:	$\dot{Q}$	heat transfer per unit time

Numerical subscripts refer to the labeled streams in the component diagram.

Turbine

Parameters

- n number of stages
- r pressure ratio per stage (input/output)
- η isentropic efficiency for each stage

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$x_{i1} = x_{i2}$$

$$p_1 = r^n \cdot p_2$$

$$\dot{W} = \dot{m}_1 \cdot (h_1 - h_2)$$

For each stage:

$$p_{in} = r \cdot p_{out}$$

$$\eta = \frac{(h_{in} - h_{out})}{(h_{in} - h_s)} \text{ where } h_s \text{ is the specific enthalpy of the fluid at } (s_{in}, p_{out}).$$

Fluid 1 is the "in" fluid for stage 1. Fluid 2 is the "out" fluid for stage n .

Notes

The fluid's chemical composition is kept frozen as the fluid flows through the turbine. However, the fluid's phase composition (liquid/gas) is allowed to change as the pressure decreases. At the turbine outlet the fluid will be in phase equilibrium, but might not be in chemical equilibrium.

Compressor

Parameters

- n number of stages
- r pressure ratio per stage (output/input)
- η isentropic efficiency for each stage

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$x_{i1} = x_{i2}$$

$$p_2 = r^n \cdot p_1$$

$$\dot{W} = \dot{m}_1 \cdot (h_2 - h_1)$$

For each stage:

$$p_{out} = r \cdot p_{in}$$

$$\eta = \frac{(h_s - h_{in})}{(h_{out} - h_{in})} \text{ where } h_s \text{ is the specific enthalpy of the fluid at } (s_{in}, p_{out}).$$

Fluid 1 is the "in" fluid for stage 1. Fluid 2 is the "out" fluid for stage n .

Notes

The fluid's chemical composition is kept frozen as the fluid flows through the compressor. However, the fluid's phase composition (liquid/gas) is allowed to change as the pressure increases. At the compressor outlet the fluid will be in phase equilibrium, but might not be in chemical equilibrium.

Heater

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$x_{i1} = x_{i2}$$

$$p_1 = p_2$$

$$\dot{Q} = \dot{m}_1 \cdot (h_2 - h_1)$$

Notes

The fluid's chemical composition is kept frozen as the fluid flows through the heater. However, the fluid's phase composition (liquid/gas) is allowed to change as the enthalpy increases. At the heater outlet the fluid will be in phase equilibrium, but might not be in chemical equilibrium.

A heater connected to a cooler with a heat connection forms a heat exchanger.

Cooler

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$x_{i1} = x_{i2}$$

$$P_1 = P_2$$

$$\dot{Q} = \dot{m}_1 \cdot (h_1 - h_2)$$

Notes

The fluid's chemical composition is kept frozen as the fluid flows through the cooler. However, the fluid's phase composition (liquid/gas) is allowed to change as the enthalpy decreases. At the cooler outlet the fluid will be in phase equilibrium, but might not be in chemical equilibrium.

A cooler connected to a heater with a heat connection forms a heat exchanger.

Perfectly Stirred Reactor (PSR)

Parameters

t residence time

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$p_1 = p_2$$

$$x_2, T_2 = PSR(x_1, p_1, T_1, t)$$

Notes

The function *PSR* predicts the steady-state temperature and species composition for a perfectly stirred reactor. It is based on a FORTRAN program named *PSR*.^a

Plug Flow Reactor (PFR)

Parameters

t residence time

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$p_1 = p_2$$

$$x_2, T_2 = PFR(x_1, p_1, T_1, t)$$

Notes

The function *PFR* predicts the steady-state temperature and species composition for a plug flow reactor. It is based on a FORTRAN program named Senkin.^b

Reformer

Parameters

ΔT equilibrium approach temperature differential

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$p_1 = p_2$$

$$\dot{Q} = \dot{m}_1 \cdot (h_2 - h_1)$$

$$x_2 = EQUIL_TP(x_1, p_2, (T_2 - \Delta T))$$

Notes

The function *EQUIL_TP* predicts the chemical equilibrium composition for a specified temperature and pressure, given an initial composition. It is based on a Chemkin implementation of the Stanjan^c solver.

The reaction that takes place in a reformer does not always proceed to completion (chemical equilibrium at T_2). Therefore, the outlet composition is approximated as the chemical equilibrium state at $(T_2 - \Delta T)$ rather than at T_2 .

P-H Equilibrator

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$p_1 = p_2$$

$$h_1 = h_2$$

$$x_2 = EQUIL_PH(x_1, p_2, h_2)$$

Notes

The P-H Equilibrator brings the fluid to chemical equilibrium at constant pressure and enthalpy.

The function *EQUIL_PH* predicts the chemical equilibrium composition for a specified enthalpy and pressure, given an initial composition. It is based on a Chemkin implementation of the Stanjan^c solver.

T-P Equilibrator

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$p_1 = p_2$$

$$T_1 = T_2$$

$$x_2 = EQUIL_TP(x_1, p_2, T_2)$$

Notes

The T-P Equilibrator brings the fluid to chemical equilibrium at constant temperature and pressure.

The function *EQUIL_TP* predicts the chemical equilibrium composition for a specified temperature and pressure, given an initial composition. It is based on a Chemkin implementation of the Stanjan^c solver.

P-H Phase Equilibrator

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$p_1 = p_2$$

$$h_1 = h_2$$

$$x_2 = PHASE_PH(x_1, p_2, h_2)$$

Notes

The P-H Phase Equilibrator brings the fluid to phase equilibrium at constant pressure and enthalpy.

The function *PHASE_PH* predicts the phase equilibrium composition for a specified enthalpy and pressure, given an initial composition. It is based on a Chemkin implementation of the Stanjan^o solver.

T-P Phase Equilibrator

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$p_1 = p_2$$

$$T_1 = T_2$$

$$x_2 = PHASE_TP(x_1, p_2, T_2)$$

Notes

The T-P Phase Equilibrator brings the fluid to phase equilibrium at constant temperature and pressure.

The function *PHASE_TP* predicts the phase equilibrium composition for a specified temperature and pressure, given an initial composition. It is based on a Chemkin implementation of the Stanjan^c solver.

Pump

Parameters

r pressure ratio (output/input)
 η efficiency

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$x_{i1} = x_{i2}$$

$$p_2 = r \cdot p_1$$

$$\dot{W} = \dot{m}_1 \cdot (h_2 - h_1)$$

$$\eta = \frac{v \cdot (p_2 - p_1)}{(h_2 - h_1)}$$

Notes

The fluid's chemical composition is kept frozen as the fluid flows through the pump. However, the fluid's phase composition (liquid/gas) is allowed to change as the pressure increases. At the pump outlet the fluid will be in phase equilibrium, but might not be in chemical equilibrium.

Valve

Parameters

r pressure ratio (input/output)

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$x_{i1} = x_{i2}$$

$$h_1 = h_2$$

$$p_1 = r \cdot p_2$$

Notes

The valve pressure reduction is isenthalpic.

The fluid's chemical composition is kept frozen as the fluid flows through the valve.

However, the fluid's phase composition (liquid/gas) is allowed to change as the pressure decreases. At the valve outlet the fluid will be in phase equilibrium, but might not be in chemical equilibrium.

Mixer (Junction)

Behavior

$$\dot{m}_1 + \dot{m}_2 = \dot{m}_3$$

$$\dot{m}_1 \cdot x_{i1} + \dot{m}_2 \cdot x_{i2} = \dot{m}_3 \cdot x_{i3}$$

$$p_3 = \min(p_1, p_2)$$

$$\dot{m}_1 \cdot h_1 + \dot{m}_2 \cdot h_2 = \dot{m}_3 \cdot h_3$$

Notes

The mixing process is adiabatic.

Splitter (Junction)

Behavior

$$\dot{m}_1 = \dot{m}_2 + \dot{m}_3$$

$$x_{i1} = x_{i2} = x_{i3}$$

$$p_1 = p_2 = p_3$$

$$h_1 = h_2 = h_3$$

Notes

The flowrate for at least one of the output fluid streams must be specified.

Separator

Behavior

$$\dot{m}_1 = \dot{m}_2 + \dot{m}_3$$

$$p_1 = p_2 = p_3$$

$$T_1 = T_2 = T_3$$

Notes

The separator component separates the incoming fluid into liquid and gas streams. The first outgoing connection created for the separator will be the gas stream, the second will be the liquid stream.

Source

Notes

The source component represents a fluid source external to the cycle.

Sink

Notes

The sink component represents a fluid sink external to the cycle.

Turbine - Frozen Composition

Parameters

- n number of stages
- r pressure ratio per stage (input/output)
- η isentropic efficiency for each stage

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$x_{i1} = x_{i2}$$

$$p_1 = r^n \cdot p_2$$

$$\dot{W} = \dot{m}_1 \cdot (h_1 - h_2)$$

For each stage:

$$p_{in} = r \cdot p_{out}$$

$$\eta = \frac{(h_{in} - h_{out})}{(h_{in} - h_s)} \text{ where } h_s \text{ is the specific enthalpy of the fluid at } (s_{in}, p_{out}).$$

Fluid 1 is the “in” fluid for stage 1. Fluid 2 is the “out” fluid for stage n .

Notes

The fluid's chemical composition and phase composition are kept frozen as fluid flows through the turbine. At the turbine outlet the fluid might not be in chemical or phase equilibrium.

Compressor - Frozen Composition

Parameters

- n number of stages
- r pressure ratio per stage (output/input)
- η isentropic efficiency for each stage

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$x_{i1} = x_{i2}$$

$$p_2 = r^n \cdot p_1$$

$$\dot{W} = \dot{m}_1 \cdot (h_2 - h_1)$$

For each stage:

$$p_{out} = r \cdot p_{in}$$

$$\eta = \frac{(h_s - h_{in})}{(h_{out} - h_{in})} \text{ where } h_s \text{ is the specific enthalpy of the fluid at } (s_{in}, p_{out}).$$

Fluid 1 is the "in" fluid for stage 1. Fluid 2 is the "out" fluid for stage n.

Notes

The fluid's chemical composition and phase composition are kept frozen as fluid flows through the compressor. At the compressor outlet the fluid might not be in chemical or phase equilibrium.

Pump - Frozen Composition

Parameters

r	pressure ratio (output/input)
η	efficiency

Behavior

$$\dot{m}_1 = \dot{m}_2$$

$$x_{i1} = x_{i2}$$

$$p_2 = r \cdot p_1$$

$$\dot{W} = \dot{m}_1 \cdot (h_2 - h_1)$$

$$\eta = \frac{v \cdot (p_2 - p_1)}{(h_2 - h_1)}$$

Notes

The fluid's chemical composition and phase composition are kept frozen as fluid flows through the pump. At the pump outlet the fluid might not be in chemical or phase equilibrium.

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