Introduction

- Typical design problems involve the determination of:
 - Overall heat transfer coefficient, e.g. for a car radiator.
 - Highest (or lowest) temperature in a system, e.g. in a gas turbine, chemical reaction vessels, food ovens.
 - Temperature distribution (related to thermal stress), e.g. in the walls of a spacecraft.
 - Temperature response in time dependent heating/cooling problems, e.g. engine cooling, or how fast does a car heat up in the sun and how is it affected by the shape of the windshield?



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Modes of heat transfer

- Conduction: diffusion of heat due to temperature gradients. A measure of the amount of conduction for a given gradient is the heat conductivity.
- Convection: when heat is carried away by moving fluid. The flow can either be caused by external influences, forced convection; or by buoyancy forces, natural convection. Convective heat transfer is tightly coupled to the fluid flow solution.
- Radiation: transfer of energy by electromagnetic waves between surfaces with different temperatures, separated by a medium that is at least partially transparent to the (infrared) radiation. Radiation is especially important at high temperatures, e.g. during combustion processes, but can also have a measurable effect at room temperatures.

Overview dimensionless numbers

- Nusselt number: $Nu = hL/k_f$. Ratio between total heat transfer in a convection dominated system and the estimated conductive heat transfer.
- Grashof number: $Gr = L^3 g \Delta \rho / v^2 \rho_w$. Ratio between buoyancy forces and viscous forces.
- Prandtl number: $Pr = \mu c_p / k$. Ratio between momentum diffusivity and thermal diffusivity. Typical values are Pr = 0.01 for liquid metals; Pr = 0.7 for most gases; Pr = 6 for water at room temperature.
- Rayleigh number: $Ra = Gr Pr = L^3 \rho^2 g \beta c_p \Delta T / \mu k = L^3 \rho g \beta \Delta T / \mu \alpha$ The Rayleigh number governs natural convection phenomena.
- Reynolds number: $Re = \rho UL / \mu$. Ratio between inertial and viscous forces.

Enthalpy equation

- In CFD it is common to solve the enthalpy equation, subject to a wide range of thermal boundary conditions.
 - Energy sources due to chemical reaction are included for reacting flows.
 - Energy sources due to species diffusion are included for multiple species flows.
 - The energy source due to viscous heating describes thermal energy created by viscous shear in the flow. This is important when the shear stress in the fluid is large (e.g. lubrication) and/or in high-velocity, compressible flows. Often, however, it is negligible.
 - In solid regions, a simple conduction equation is usually solved, although convective terms can also be included for moving solids.

Conjugate heat transfer

- "Conjugate heat transfer" refers to the ability to compute conduction of heat through solids, coupled with convective heat transfer in a fluid.
- Coupled boundary conditions are available for wall zones that separate two cell zones.
- Either the solid zone or the fluid zone, or both, may contain heat sources.
- The example here shows the temperature profile for coolant flowing over fuel rods that generate heat.



Temperature contours

Example: Cooling flow over fuel rods

Periodic heat transfer

- Also known as streamwise-periodic or fully-developed flow.
- Used when flow and heat transfer patterns are repeated, e.g.
 - Compact heat exchangers.
 - Flow across tube banks.
- Geometry and boundary conditions repeat in streamwise direction.



Heat conduction - Fourier's law

• The heat flux is proportional to the temperature gradient:

$$\frac{Q}{A} = q = -k\nabla T$$

where k(x,y,z,T) is the thermal conductivity.

 In most practical situations conduction, convection, and radiation appear in combination. Also for convection, the heat transfer coefficient is important, because a flow can only carry heat away from a wall when that wall is conducting.



Generalized heat diffusion equation

• If we perform a heat balance on a small volume of material....



• ... we get:

$$\rho c \frac{\partial T}{\partial t} = k \nabla^2 T + \dot{q}$$



Conduction example

• Compute the heat transfer through the wall of a home:



Convection heat transfer

- Convection is movement of heat with a fluid.
- E.g., when cold air sweeps past a warm body, it draws away warm air near the body and replaces it with cold air.



Forced convection example

• Developing flow in a pipe (constant wall temperature).



Thermal boundary layer

- Just as there is a viscous boundary layer in the velocity distribution, there is also a thermal boundary layer.
- Thermal boundary layer thickness is different from the thickness of the (momentum) viscous sublayer, and fluid dependent. The thickness of the thermal sublayer for a high-Prandtl-number fluid (e.g. water) is much less than the momentum sublayer thickness. For fluids of low Prandtl numbers (e.g. liquid metal), it is much larger than the momentum sublayer thickness.



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Natural convection

- Natural convection (from a heated vertical plate).
- As the fluid is warmed by the plate, its density decreases and a buoyant force arises which induces flow in the vertical direction. The force is proportional to $(\rho \rho_{\infty})g$.
- The dimensionless group that governs natural convection is the Rayleigh number:

$$Ra = Gr.Pr = \frac{g\beta\Delta TL^3}{\alpha\upsilon}$$

• Typically: $Nu \propto Ra^x$ $\frac{1}{4} < x < \frac{1}{3}$



Natural convection around a person

- Light weight warm air tends to move upward when surrounded by cooler air.
- Thus, warm-blooded animals are surrounded by thermal plumes of rising warm air.
- This plume is made visible by means of a Schlieren optical system that is based on the fact that the refraction of light through a gas is dependent on the density of the gas.
- Although the velocity of the rising air is relatively small, the Reynolds number for this flow is on the order of 3000.



Natural convection - Boussinesq model

- Makes simplifying assumption that density is uniform.
 - Except for the body force term in the momentum equation, which is replaced by:

$$(\rho - \rho_0)g = -\rho_0\beta(T - T_0)g$$

- Valid when density variations are small (i.e. small variations in T).
- Provides faster convergence for many natural-convection flows than by using fluid density as function of temperature because the constant density assumptions reduces non-linearity.
- Natural convection problems inside closed domains:
 - For steady-state solver, Boussinesq model must be used. Constant density ρ_o allows mass in volume to be defined.
 - For unsteady solver, Boussinesq model or ideal gas law can be used. Initial conditions define mass in volume.

Newton's law of cooling

- Newton described the cooling of objects with an arbitrary shape in a pragmatic way. He postulated that the heat transfer Q is proportional to the surface area A of the object and a temperature difference ΔT.
- The proportionality constant is the heat transfer coefficient h(W/m²-K). This empirical constant lumps together all the information about the heat transfer process that we don't know or don't understand.



Heat transfer coefficient

- *h* is not a constant, but $h = h(\Delta T)$.
- Three types of convection.
- Natural convection. Fluid moves due to buoyancy.

 $h \propto \Delta T^x$ $\frac{1}{4} < x < \frac{1}{3}$

• Forced convection: flow is induced by external means.

h = const

 Boiling convection: body is hot enough to boil liquid.

 $h \propto \Delta T^2$



Radiation heat transfer

- Thermal radiation is emission of energy as electromagnetic waves.
- Intensity depends on body temperature and surface characteristics.
- Important mode of heat transfer at high temperatures, e.g. combustion.
- Can also be important in natural convection problems.
- Radiation properties can be strong functions of chemical composition, especially CO₂, H₂O.
- Radiation heat exchange is difficult solve (except for simple configurations). We must rely on computational methods.

Surface characteristics



Black body radiation

- A "black body":
 - Is a model of a perfect radiator.
 - Absorbs all energy that reaches it; reflects nothing.
 - Therefore $\alpha = 1$, $\Re = \tau = 0$.
- The energy emitted by a black body is the theoretical maximum:

$$q = \sigma T^2$$

- This is Stefan-Boltzmann law; σ is the Stefan-Boltzmann constant (5.6697E-8 W/m²K⁴).
- The wavelength at which the maximum amount of radiation occurs is given by Wien's law: $\lambda_{max} T = 2.898E 3 [mK]$
- Typical wavelengths are $\lambda_{max} = 10 \ \mu m$ (far infrared) at room temperature and $\lambda_{max} = 0.5 \ \mu m$ (green) at 6000K.

Real bodies

- Real bodies will emit less radiation than a black body: $q = arepsilon \sigma T^4$
- Here *ɛ* is the emissivity, which is a number between 0 and 1.
 Such a body would be called "gray" because the emissivity is the average over the spectrum.
- Example: radiation from a small body to its surroundings.
 - Both the body and its surroundings emit thermal radiation.
 - The net heat transfer will be from the hotter to the colder.
- The net heat transfer is then: $Q_{net} = \varepsilon A \sigma (T_w^4 T_\infty^4)$
- For small ΔT the term $(T_w^4 T_\infty^4)$ can be approximated as $4\overline{T}^3(T_w - T_\infty)$ and $Q_{net} = Ah_r \Delta T$ with h_r as an effective radiation heat transfer coefficient.



The radiative heat transfer equation (RTE)

$$\frac{dI(\vec{r},\vec{s})}{ds} + (a + \sigma_s)I(\vec{r},\vec{s}) = an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(\vec{r},\vec{s}\,') \,\,\Phi(\vec{s}\cdot\vec{s}\,') \,\,d\Omega'$$

where \vec{r} = position vector = direction vector \vec{s} $\vec{s}' = \text{scattering direction vector}$ = path length S = absorption coefficient а = refractive index n σ_s = scattering coefficient σ = Stefan-Boltzmann constant (5.672 × 10⁻⁸ W/m²-K⁴) = radiation intensity, which depends on position (\vec{r}) Ι and direction (\vec{s}) T = local temperature Φ = phase function Ω' = solid angle

 $(a + \sigma_s)s$ is the optical thickness or opacity of the medium. The refractive index *n* is important when considering radiation in semi-transparent media.

Radiation

- Radiation intensity transport equations (RTE) are solved.
 - Local absorption by fluid and at boundaries links energy equation with RTE.
- Radiation intensity is directionally and spatially dependent.
 - Intensity along any direction can be reduced by:
 - Local absorption.
 - Out-scattering (scattering away from the direction).
 - Intensity along any direction can be augmented by:
 - Local emission.
 - In-scattering (scattering into the direction).
- Four common radiation models are:
 - Discrete Ordinates Model (DOM).
 - Discrete Transfer Radiation Model (DTRM).
 - P-1 Radiation Model.
 - Rosseland Model.



Discrete ordinates model

 The radiative transfer equation is solved for a discrete number of finite solid angles:

$$\frac{\partial I_{s_i}}{\partial x_i} + (a + \sigma_s)I(r, s) = an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_{0}^{4\pi} I(r, s')\Phi(s \cdot s')d\Omega'$$
absorption
emission
emission
emission
emission
emission

- Advantages:
 - Solution method similar to that for the other conservation equations.
 - Conservative method leads to heat balance for coarse discretization.
 - Accuracy can be increased by using a finer discretization.
 - Accounts for scattering, semi-transparent media, specular surfaces.
 - Banded-gray option for wavelength-dependent transmission.
- Limitations:
 - Solving a problem with a large number of ordinates is CPU-intensive.

Discrete transfer radiation model (DTRM)

- Main assumption: radiation leaving surface element in a specific range of solid angles can be approximated by a single ray.
- Uses ray-tracing technique to integrate radiant intensity along each ray:

$$\frac{dI}{ds} = -\alpha I + \alpha \frac{\sigma T^4}{\pi}$$

- Advantages:
 - Relatively simple model.
 - Can increase accuracy by increasing number of rays.
 - Applies to wide range of optical thicknesses.
- Limitations:
 - Assumes all surfaces are diffuse (isotropic reflection).
 - Effect of scattering not included.
 - Solving a problem with a large number of rays is CPU-intensive.

P-1 model

- Main assumption: radiation intensity can be decomposed into series of spherical harmonics. Only first term in this (rapidly converging) series used in P-1 model.
- Advantages:
 - Radiative transfer equation easy to solve with little CPU demand.
 - Works reasonably well for combustion applications where optical thickness is large.
 - Easily applied to complicated geometries with curvilinear coordinates.
 - Effects of particles, droplets, and soot can be included.
- Limitations:
 - Assumes all surfaces are diffuse.
 - May result in loss of accuracy, depending on complexity of geometry, if optical thickness is small.
 - Tends to overpredict radiative fluxes from localized heat sources or sinks.
- A further simplified (and faster but less accurate) version of this model is the Rosseland model.

Choosing a radiation model

- For certain problems, one radiation model may be more appropriate in general.
 - Computational effort: P-1 gives reasonable accuracy with less effort.
 - Accuracy: DTRM and DOM more accurate.
 - Optical thickness: DTRM/DOM for optically thin media (optical thickness << 1); P-1 sufficiently accurate and faster for optically thick media.
 - Scattering: P-1 and DOM account for scattering.
 - Particulate effects: P-1 and DOM account for radiation exchange between gas and particulates.
 - Localized heat sources: DTRM/DOM with sufficiently large number of rays/ordinates is more appropriate.
- DOM is the only model that works across the full range of conditions.

Wall heat flux calculation

heat flux :
$$q = h_f (T_w - T_f) + q_{rad}$$

for laminar flows : $h_f = \frac{k_f}{\Delta y}$

for turbulent flows: h_f follows from correlations describing

the thermal boundary layer profile

external wall radiation: $q_{rad} = \varepsilon_{ext} \sigma (T_{\infty}^4 - T_{w}^4)$

 $T_w =$ wall temperature

 $T_f =$ fluid cell temperature

 T_{∞} = user specified temperature

 ε_{ext} = emissivity of external wall surface

 $\sigma =$ Stefan – Boltzmann constant

 $h_f =$ fluid side local heat transfer coefficient

 $\Delta y =$ normal distance fluid cell center to wall

Heat transfer optimization

- We have the following relations for heat transfer:
 - Conduction: $Q = A \Delta T k_f / d$
 - Convection: $Q = Ah\Delta T$
 - Radiation: $Q = A h_r \Delta T$
- As a result, when equipment designers want to improve heat transfer rates, they focus on:
 - Increasing the area A, e.g. by using profiled pipes and ribbed surfaces.
 - Increasing ΔT (which is not always controllable).
 - For conduction, increasing k_f/d .
 - Increase *h* by not relying on natural convection, but introducing forced convection.
 - Increase h_r , by using "black" surfaces.

Fluid properties

- Fluid properties such as heat capacity, conductivity, and viscosity can be defined as:
 - Constant.
 - Temperature-dependent.
 - Composition-dependent.
 - Computed by kinetic theory.
 - Computed by user-defined functions.
- Density can be computed by ideal gas law.
- Alternately, density can be treated as:
 - Constant (with optional Boussinesq modeling).
 - Temperature-dependent.
 - Composition-dependent.
 - User defined functions.

Phase change

- Systems in which phase change occurs (e.g. melting, solidification, and sometimes evaporation) can be modeled as a single-phase flow with modified physical properties.
- In that case, the medium gets the properties of one phase state below a certain critical temperature, and the properties of the other phase state above a second critical temperature.
- Linear transitions for μ and ρ .
- A "spike" in c_p is added, the area of which corresponds to the latent heat.



 A second spike is added to the heat conductivity curve, to keep the ratio between heat capacity and thermal conductivity constant.

Thermal boundary conditions

- At flow inlets and exits.
 - At flow inlets, must supply fluid temperature.
 - At flow exits, fluid temperature extrapolated from upstream value.
 - At pressure outlets, where flow reversal may occur, "backflow" temperature is required.
- Thermal conditions for fluids and solids.
 - Can specify energy source.
- Thermal boundary conditions at walls.
 - Specified heat flux.
 - Specified temperature.
 - Convective heat transfer.
 - External radiation.
 - Combined external radiation and external convective heat transfer.

Notes on convergence

- Heat transfer calculations often converge slowly. It is recommended to use underrelaxation factors of 0.9 or larger for enthalpy. If lower underrelaxation factors are used, obtaining a good solution may take prohibitively long.
- If underrelaxation factors of 0.2 or lower have to be used to prevent divergence, it usually means that the model is ill-posed.
- Deep convergence is usually required with scaled residuals having to be of the order 1E-6 or smaller.

Example: heat exchanger efficiency

- Problem: improve the efficiency of a tube-cooled reactor.
- Non-standard design, i.e. traditional correlation based methods not applicable.
- Solution: more uniform flow distribution through the shell that will result in a higher overall heat transfer coefficient and improved efficiency.



Heat exchanger - original design



Heat exchanger - modeling approach

- 3-dimensional, steady, turbulent, incompressible, isothermal.
- Bundle of tubes modeled as a non-isotropic porous medium. Two symmetry planes significantly reduce domain size.
- Hybrid, unstructured mesh of 330,000 cells.
- Zero thickness walls for baffles.
- Leakage between baffles and shell wall (0.15" gap) modeled using thin prism cells.
- Uniform inflow applied over a half-cylindrical surface upstream of the first baffle.



Heat exchanger - flow pattern



Non-uniform flow distribution means low efficiency

Heat exchanger - modifications



Heat exchanger - improved flow pattern

- Flow distribution after modifications.
- No recirculating fluid between baffles C' and A.
- Almost uniform flow distribution.
- Problem has unique flow arrangement that does not allow traditional methods to be of any help.
- A simplified CFD model leads to significantly improved performance of the heat exchanger/reactor.



Conclusion

- Heat transfer is the study of thermal energy (heat) flows: conduction, convection, and radiation.
- The fluid flow and heat transfer problems can be tightly coupled through the convection term in the energy equation and when physical properties are temperature dependent.
- Chemical reactions, such as combustion, can lead to source terms to be included in the enthalpy equation.
- While analytical solutions exist for some simple problems, we must rely on computational methods to solve most industrially relevant applications.