ThermophysicalModels library in OpenFOAM-2.3.x

How to implement a new thermophysical model

Teaching within: CFD with OpenSource software (TME050)

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Exemples of thermodynamic and transport properties:

- density ρ → *equation of state (Ia, see slide 4)*
- heat capacity C_v , C_p
- internal energy e, enthalpy h

→ *thermophysical properties (Ib, see slide 5)*

- diffusivity D,α …
- viscosity μ
- thermal conductivity κ
- electric conductivity

→ *transport properties (Ic, see slide 6)*

Depend on:

- temperature T
- pressure P

→ *Pure mixture (Ia-Ic, see slide 4-6)*

- fluid (possibly solid) composition → *Mixture (II, see slide 7)*

Involved in heat transfer, compressible flow, multiphase problems, combustion, etc.

Content

Slides

Models available in OpenFOAM (see UserGuide) *(1/8)*

Ia

Equation of State — equationOfState	
adiabaticPerfectFluid	Adiabatic perfect gas equation of state
icoPolynomial	Incompressible polynomial equation of state, *e.g.* for liquids
perfectFluid	Perfect gas equation of state
incompressiblePerfectGas	Incompressible gas equation of state using a constant reference pressure. Density only varies with temperature and composition
rhoConst	Constant density equation of state

Models available in OpenFOAM (see UserGuide) *(2/8)*

Ib Basic thermophysical properties — thermo

eConstThermo	Constant specific heat c_p model with evaluation of internal energy e and entropy s
hConstThermo	Constant specific heat c_p model with evaluation of enthalpy h and entropy s
hPolynomialThermo	c_p evaluated by a function with coefficients from polynomials, from which h, s are evaluated
janafThermo	c_p evaluated by a function with coefficients from JANAF thermodynamic tables, from which h, s are evaluated

Models available in OpenFOAM (see UserGuide) *(3/8)*

Ic

Transport properties — transport	
constTransport	Constant transport properties
polynomialTransport	Polynomial based temperature-dependent transport properties
sutherlandTransport	Sutherland's formula for temperature-dependent transport properties

Models available in OpenFOAM (see UserGuide) *(4/8)*

II Mixture properties — mixture

pureMixture	General thermophysical model calculation for passive gas mixtures
homogeneousMixture	Combustion mixture based on normalised fuel mass fraction b
inhomogeneousMixture	Combustion mixture based on b and total fuel mass fraction f_t
veryInhomogeneousMixture	Combustion mixture based on b, f_t and unburnt fuel mass fraction f_u
basicMultiComponent-Mixture	Basic mixture based on multiple components
multiComponentMixture	Derived mixture based on multiple components
reactingMixture	Combustion mixture using thermodynamics and reaction schemes
egrMixture	Exhaust gas recirculation mixture
singleStepReactingMixture	Single step reacting mixture

→ **Ia, Ib & Ic**

→ **Ia, Ib & Ic** for all species **&** suited mixing rules

Models available in OpenFOAM (see UserGuide) *(5/8)*

III Thermophysical model — thermoModel **Combines Ia, Ib, Ic & II**

hePsiThermo	General thermophysical model calculation based on compressibility ψ
heRhoThermo	General thermophysical model calculation based on density ρ
psiReactionThermo	Calculates enthalpy for combustion mixture based on ψ
psiuReactionThermo	Calculates enthalpy for combustion mixture based on ψ_u
rhoReactionThermo	Calculates enthalpy for combustion mixture based on ρ
heheupsiReactionThermo	Calculates enthalpy for unburnt gas and combustion mixture

Models available in OpenFOAM (for a given solver) *(6/8)*

Example: go to tuturials/heatTransfer/buoyantSimpleFoam/buoyantCavity/constant
in thermophysicalProperties change ”transport const” to ”transport dummy”
and run the solver buoyantSimpleFoam;
it returns the list of thermophysical models available for this solver:

```
Valid rhoThermo types are:

type  III    mixture  II                transport  thermo      equationOfState          specie  energy

heRhoThermo  homogeneousMixture        const      hConst      incompressiblePerfectGas specie  sensibleEnthalpy
heRhoThermo  homogeneousMixture        const      hConst      perfectGas               specie  sensibleEnthalpy
heRhoThermo  homogeneousMixture        sutherland janaf       incompressiblePerfectGas specie  sensibleEnthalpy
heRhoThermo  homogeneousMixture        sutherland janaf       perfectGas               specie  sensibleEnthalpy
heRhoThermo  inhomogeneousMixture      const      hConst      incompressiblePerfectGas specie  sensibleEnthalpy
heRhoThermo  inhomogeneousMixture      const      hConst      perfectGas               specie  sensibleEnthalpy
```

Ic Ib Ia

… (+ 2 following slides)

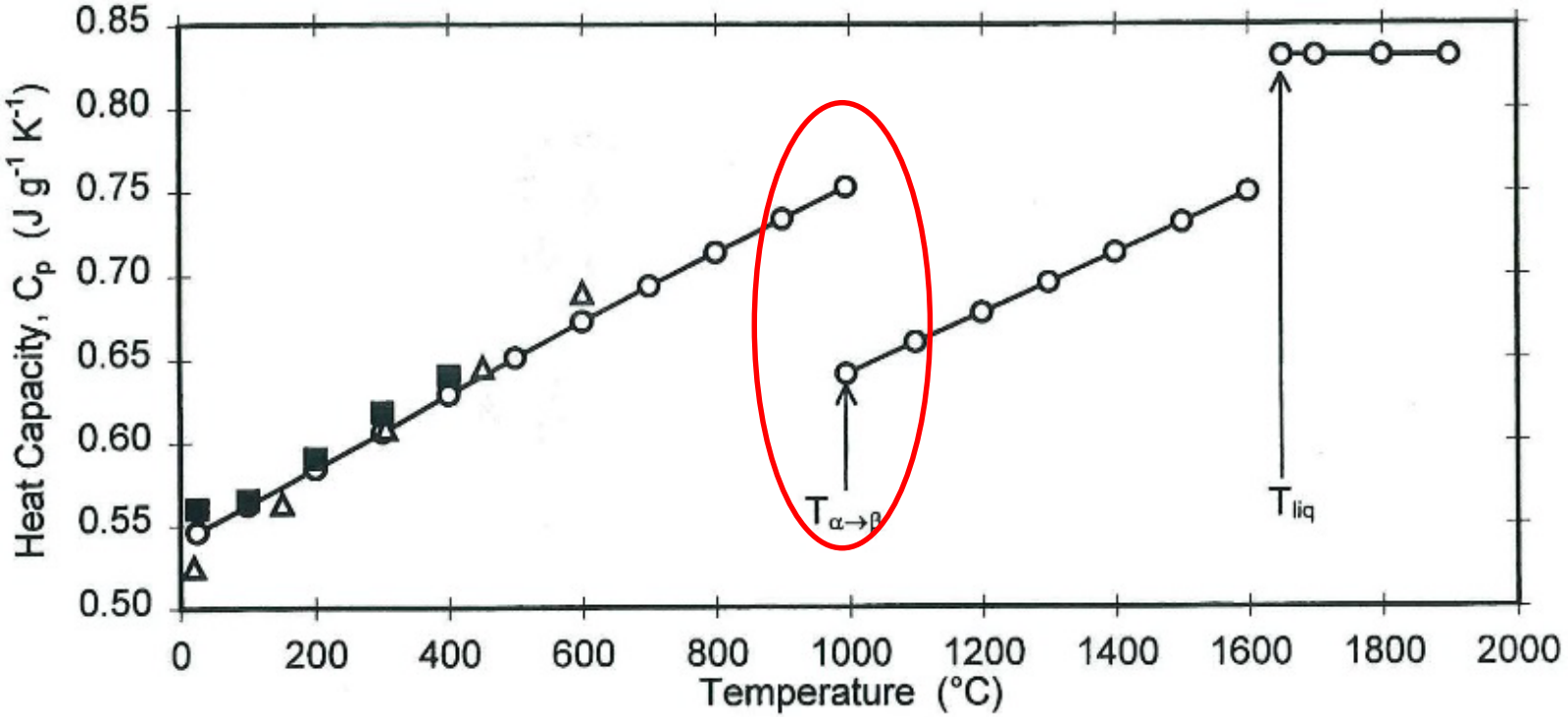
Models available in OpenFOAM (for a given solver) *(7/8)*

heRhoThermo	inhomogeneousMixture	sutherland	janaf	incompressiblePerfectGas	specie	sensibleEnthalpy
heRhoThermo	inhomogeneousMixture	sutherland	janaf	perfectGas	specie	sensibleEnthalpy
heRhoThermo	multiComponentMixture	const	hConst	incompressiblePerfectGas	specie	sensibleEnthalpy
heRhoThermo	multiComponentMixture	const	hConst	incompressiblePerfectGas	specie	sensibleInternalEnergy
heRhoThermo	multiComponentMixture	const	hConst	perfectGas	specie	sensibleEnthalpy
heRhoThermo	multiComponentMixture	const	hConst	perfectGas	specie	sensibleInternalEnergy
heRhoThermo	multiComponentMixture	polynomial	hPolynomial	icoPolynomial	specie	sensibleEnthalpy
heRhoThermo	multiComponentMixture	polynomial	hPolynomial	icoPolynomial	specie	sensibleInternalEnergy
heRhoThermo	multiComponentMixture	sutherland	janaf	incompressiblePerfectGas	specie	sensibleEnthalpy
heRhoThermo	multiComponentMixture	sutherland	janaf	incompressiblePerfectGas	specie	sensibleInternalEnergy
heRhoThermo	multiComponentMixture	sutherland	janaf	perfectGas	specie	sensibleEnthalpy
heRhoThermo	multiComponentMixture	sutherland	janaf	perfectGas	specie	sensibleInternalEnergy
heRhoThermo	pureMixture	const	hConst	adiabaticPerfectFluid	specie	sensibleEnthalpy
heRhoThermo	pureMixture	const	hConst	adiabaticPerfectFluid	specie	sensibleInternalEnergy
heRhoThermo	pureMixture	const	hConst	incompressiblePerfectGas	specie	sensibleEnthalpy
heRhoThermo	pureMixture	const	hConst	incompressiblePerfectGas	specie	sensibleInternalEnergy
heRhoThermo	pureMixture	const	hConst	perfectFluid	specie	sensibleEnthalpy
heRhoThermo	pureMixture	const	hConst	perfectFluid	specie	sensibleInternalEnergy
heRhoThermo	pureMixture	const	hConst	perfectGas	specie	sensibleEnthalpy
heRhoThermo	pureMixture	const	hConst	perfectGas	specie	sensibleInternalEnergy
heRhoThermo	pureMixture	const	hConst	rhoConst	specie	sensibleEnthalpy
heRhoThermo	pureMixture	const	hConst	rhoConst	specie	sensibleInternalEnergy
heRhoThermo	pureMixture	kineticAr	hKineticAr	rhoKineticAr	specie	sensibleEnthalpy
heRhoThermo	pureMixture	polynomial	hPolynomial	PengRobinsonGas	specie	sensibleEnthalpy
heRhoThermo	pureMixture	polynomial	hPolynomial	icoPolynomial	specie	sensibleEnthalpy
heRhoThermo	pureMixture	polynomial	hPolynomial	icoPolynomial	specie	sensibleInternalEnergy

Models available in OpenFOAM (for a given solver) *(8/8)*

heRhoThermo	pureMixture	polynomial	janaf	PengRobinsonGas	specie	sensibleEnthalpy
heRhoThermo	pureMixture	sutherland	hConst	PengRobinsonGas	specie	sensibleEnthalpy
heRhoThermo	pureMixture	sutherland	hConst	incompressiblePerfectGas	specie	sensibleEnthalpy
heRhoThermo	pureMixture	sutherland	hConst	incompressiblePerfectGas	specie	sensibleInternalEnergy
heRhoThermo	pureMixture	sutherland	hConst	perfectGas	specie	sensibleEnthalpy
heRhoThermo	pureMixture	sutherland	hConst	perfectGas	specie	sensibleInternalEnergy
heRhoThermo	pureMixture	sutherland	janaf	incompressiblePerfectGas	specie	sensibleEnthalpy
heRhoThermo	pureMixture	sutherland	janaf	incompressiblePerfectGas	specie	sensibleInternalEnergy
heRhoThermo	pureMixture	sutherland	janaf	perfectGas	specie	sensibleEnthalpy
heRhoThermo	pureMixture	sutherland	janaf	perfectGas	specie	sensibleInternalEnergy
heRhoThermo	reactingMixture	const	hConst	incompressiblePerfectGas	specie	sensibleEnthalpy
heRhoThermo	reactingMixture	const	hConst	incompressiblePerfectGas	specie	sensibleInternalEnergy
heRhoThermo	reactingMixture	const	hConst	perfectGas	specie	sensibleEnthalpy
heRhoThermo	reactingMixture	const	hConst	perfectGas	specie	sensibleInternalEnergy
heRhoThermo	reactingMixture	polynomial	hPolynomial	icoPolynomial	specie	sensibleEnthalpy
heRhoThermo	reactingMixture	polynomial	hPolynomial	icoPolynomial	specie	sensibleInternalEnergy
heRhoThermo	reactingMixture	sutherland	janaf	incompressiblePerfectGas	specie	sensibleEnthalpy
heRhoThermo	reactingMixture	sutherland	janaf	incompressiblePerfectGas	specie	sensibleInternalEnergy
heRhoThermo	reactingMixture	sutherland	janaf	perfectGas	specie	sensibleEnthalpy
heRhoThermo	reactingMixture	sutherland	janaf	perfectGas	specie	sensibleInternalEnergy
heRhoThermo	singleStepReactingMixture	sutherland	janaf	perfectGas	specie	sensibleEnthalpy
heRhoThermo	singleStepReactingMixture	sutherland	janaf	perfectGas	specie	sensibleInternalEnergy
heRhoThermo	veryInhomogeneousMixture	const	hConst	incompressiblePerfectGas	specie	sensibleEnthalpy
heRhoThermo	veryInhomogeneousMixture	const	hConst	perfectGas	specie	sensibleEnthalpy
heRhoThermo	veryInhomogeneousMixture	sutherland	janaf	incompressiblePerfectGas	specie	sensibleEnthalpy
heRhoThermo	veryInhomogeneousMixture	sutherland	janaf	perfectGas	specie	sensibleEnthalpy

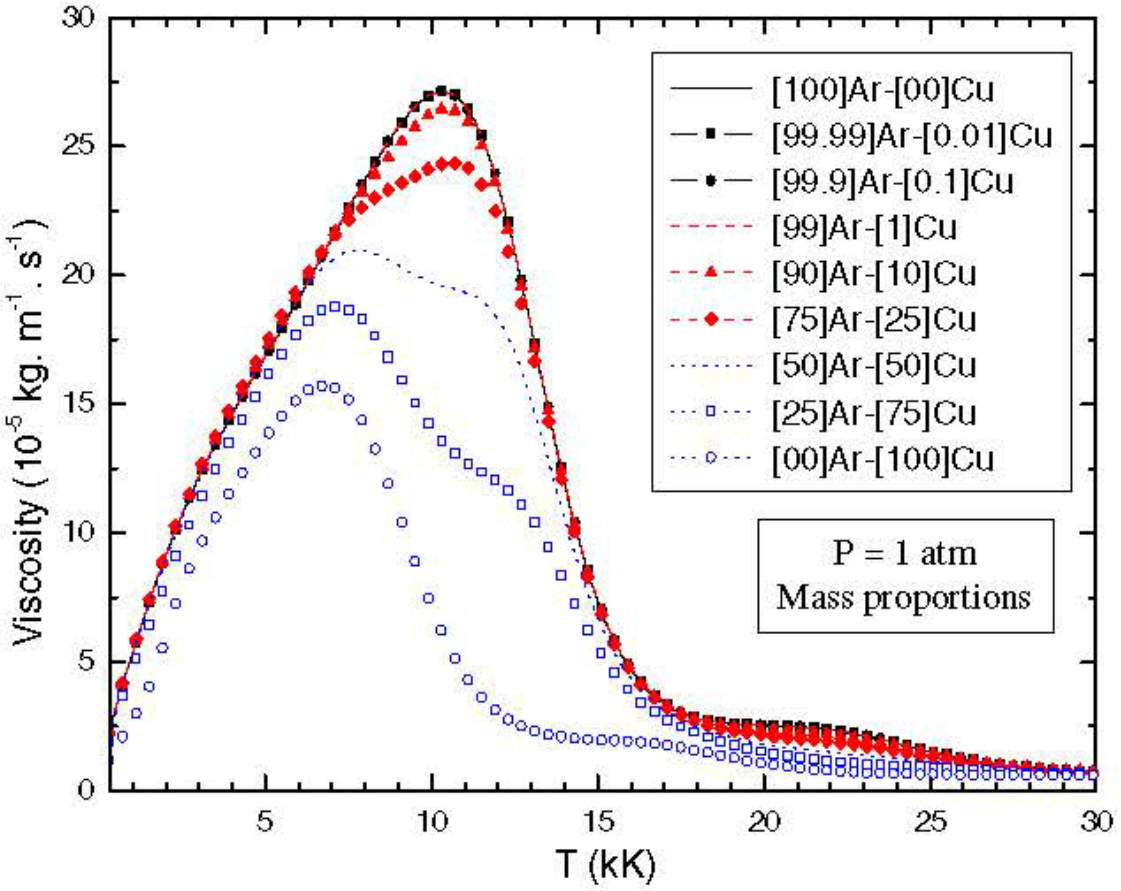
Other example of thermophysical model : *phase change in solid state* *(1/3)*



Heat capacity of Ti/6Al/4V as a function of temperature; ——, o, recommended values; Δ, Bros [3]; ■, Richardson [4].

From "Recommended values of thermophysical properties for selected commetcial alloys", Kenneth C Mills, ASM International, ISBN 0-87170-753-5, (page 213)

Other example of thermophysical model : *thermal plasma* *(2/3)*



Viscosity of Ar–Cu mixtures at atmospheric pressure.

From “Thermal plasma properties for Ar–Cu, Ar–Fe and Ar–Al mixtures used in welding plasmas processes: II. Transport coefficients at atmospheric pressure”, Y Cressault, A B Murphy, Ph Teulet, A Gleizes and M Schnick, J. Phys. D: Appl. Phys. **46** (2013) 415207

Other example of thermophysical model : *thermal plasma* *(3/3)*

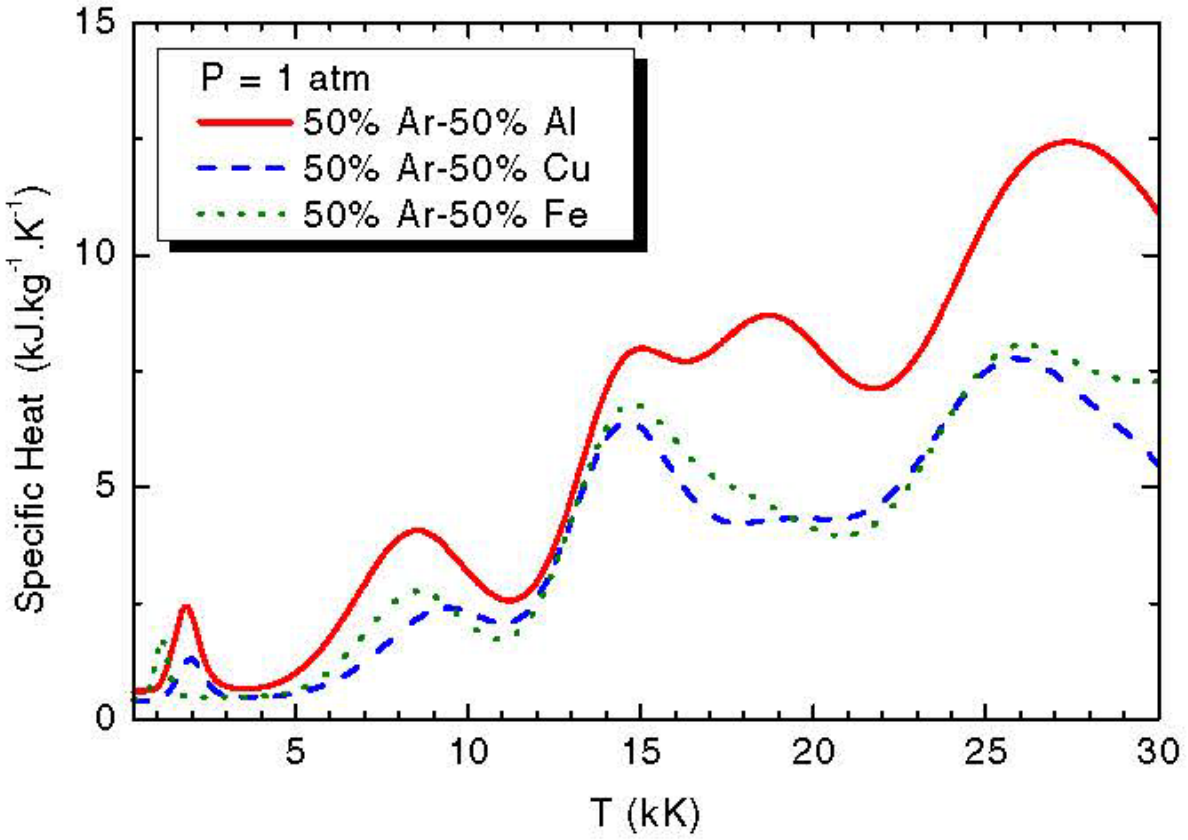


Figure 1. Specific heat at constant pressure for 50%Ar–50% metal vapour mixtures by mass at atmospheric pressure.

From “Thermal plasma properties for Ar–Cu, Ar–Fe and Ar–Al mixtures used in welding plasmas processes: II. Transport coefficients at atmospheric pressure”, Y Cressault, A B Murphy, Ph Teulet, A Gleizes and M Schnick, J. Phys. D: Appl. Phys. **46** (2013) 415207

Example of problem needing a new thermophysical model : *(1/16)*

thermal conduction in a high temperature argon gas

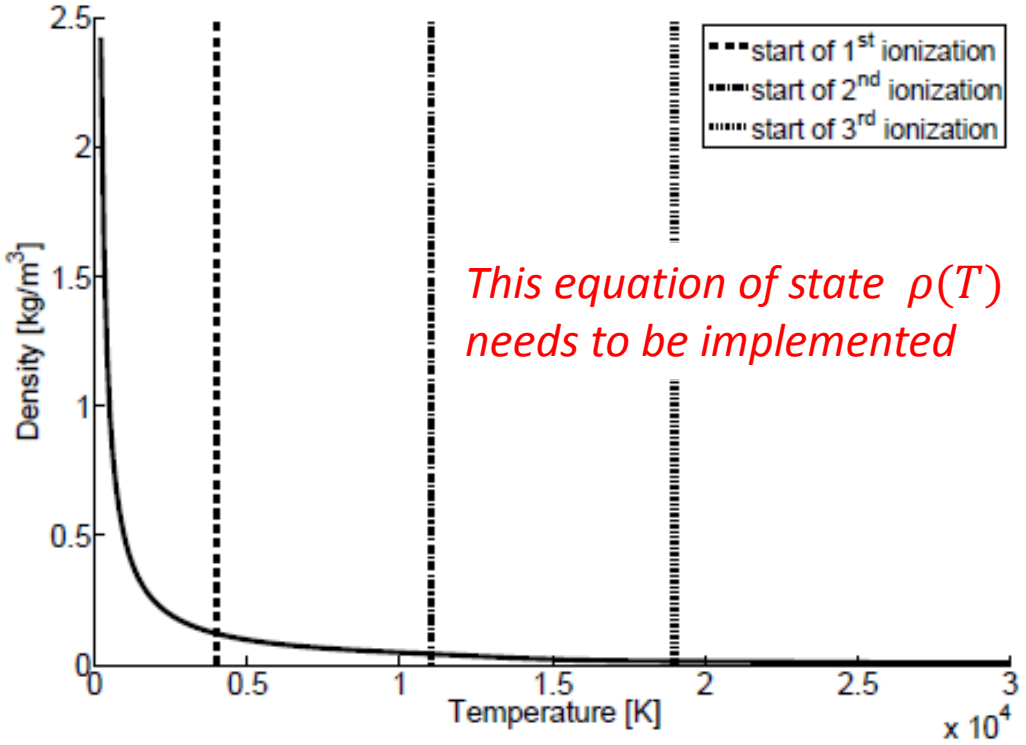
Governing equation

$$\frac{\partial(\rho\, C_v T)}{\partial t} = \nabla(\kappa\, \nabla.T)$$

with ρ, C_v and κ function of T obtained

from kinetic theory for $T \in [200; 20000]K$

Rk: need a heatTransfer solver



This equation of state $\rho(T)$ needs to be implemented

Figure 2.2: Density of an argon gas versus temperature .

From "Plasma arc welding simulation with openFOAM", M. Sass-Tisovskaya, Lic. thesis, Dept. Applied Mechanics, Chalmers University of Technology, 2009 (page 30)

Example of problem needing a new thermophysical model : *(2/16)*

thermal conduction in a high temperature argon gas

This thermodynamic property
$C_p(T)$ needs to be implemented

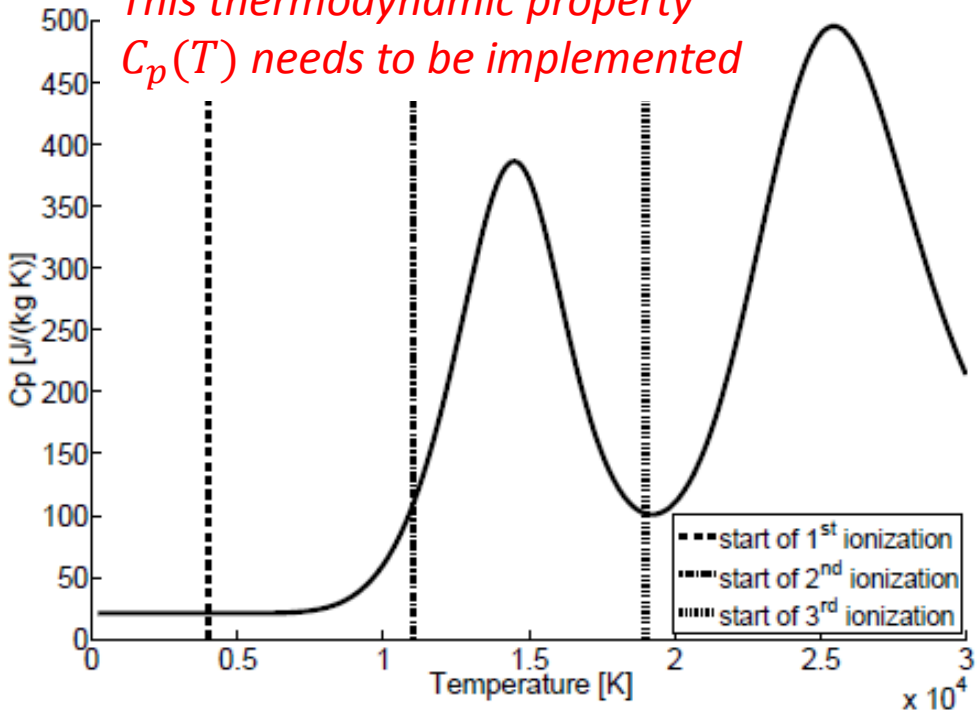


Figure 2.5: Heat capacity at constant pressure of an argon gas versus temperature.

This transport property
$\kappa(T)$ needs to be implemented

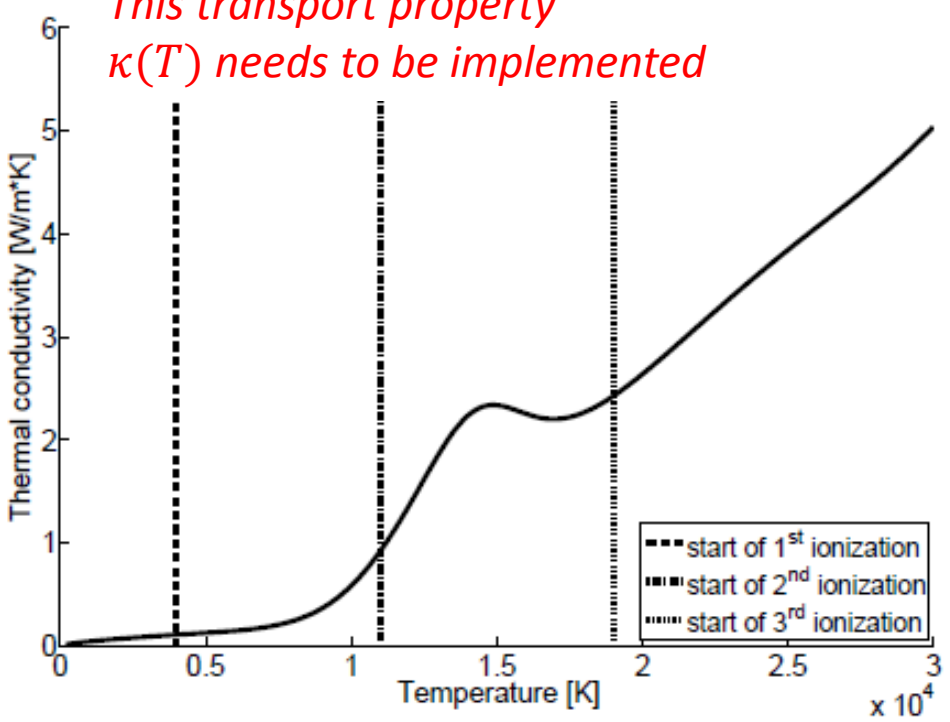


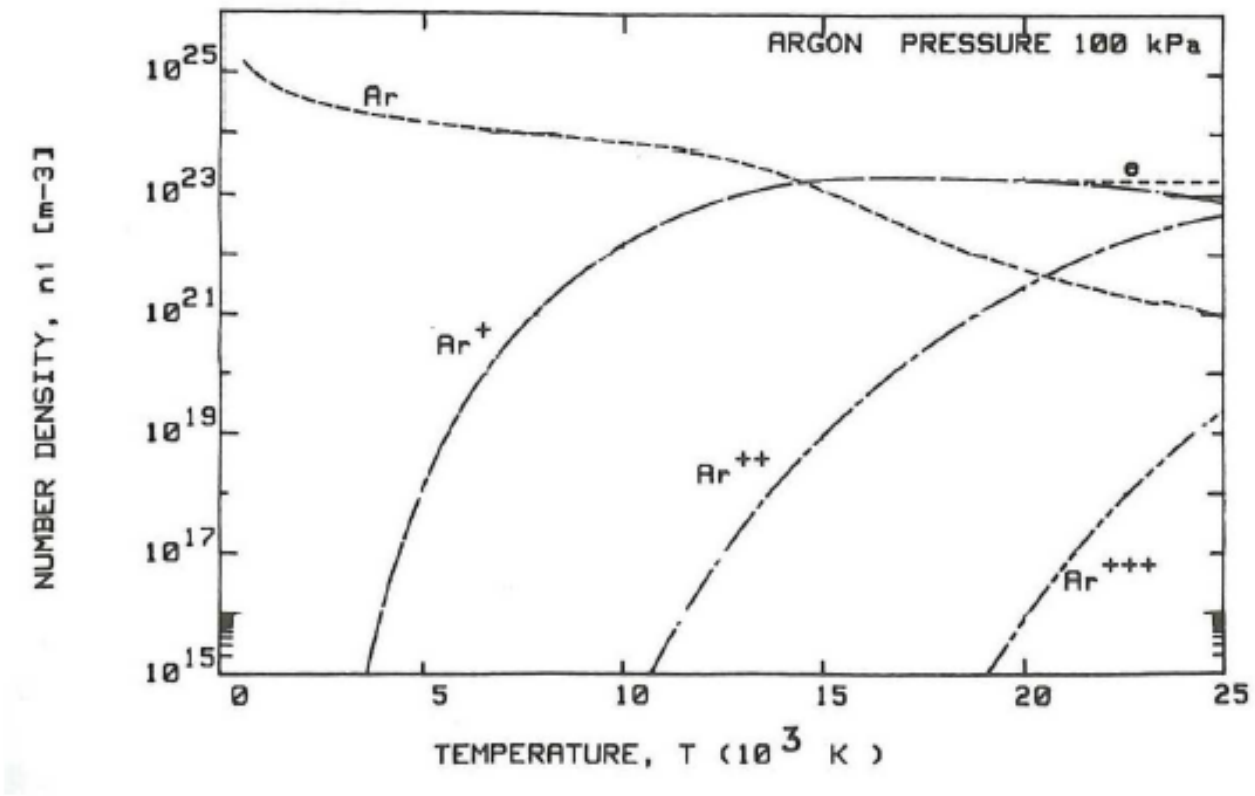
Figure 2.4: Thermal conductivity of an argon gas versus temperature.

From "Plasma arc welding simulation with openFOAM", M. Sass-Tisovskaya,
Lic. thesis, Dept. Applied Mechanics, Chalmers University of Technology, 2009 (page 31)

Example of problem needing a new thermophysical model : *(3/16)*

thermal conduction in a high temperature argon gas

Why these peaks in C_p and κ ? Because the fluid is not a pure substance: its composition changes with T.



Temperature dependence of the equilibrium composition (species number densities) of an argon plasma at atmospheric pressure (starting from one mole of Ar at room temperature [21].)

From "Thermal Plasmas, Fundamentals and Applications", Boulos M.I., Fauchais P. and Pfender E.: Vol. 1, Plenum Press, New York, 1994 (page 235)

Example of problem needing a new thermophysical model : *(4/16)*

thermal conduction in a high temperature argon gas

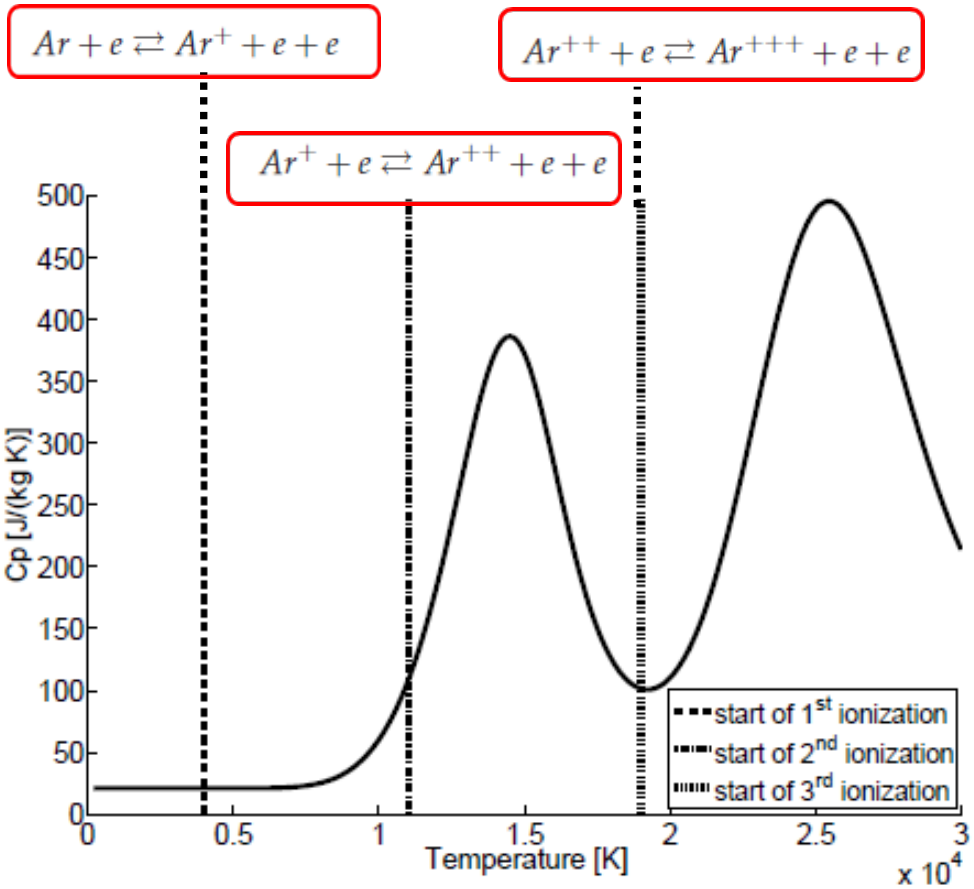


Figure 2.5: Heat capacity at constant pressure of an argon gas versus temperature.

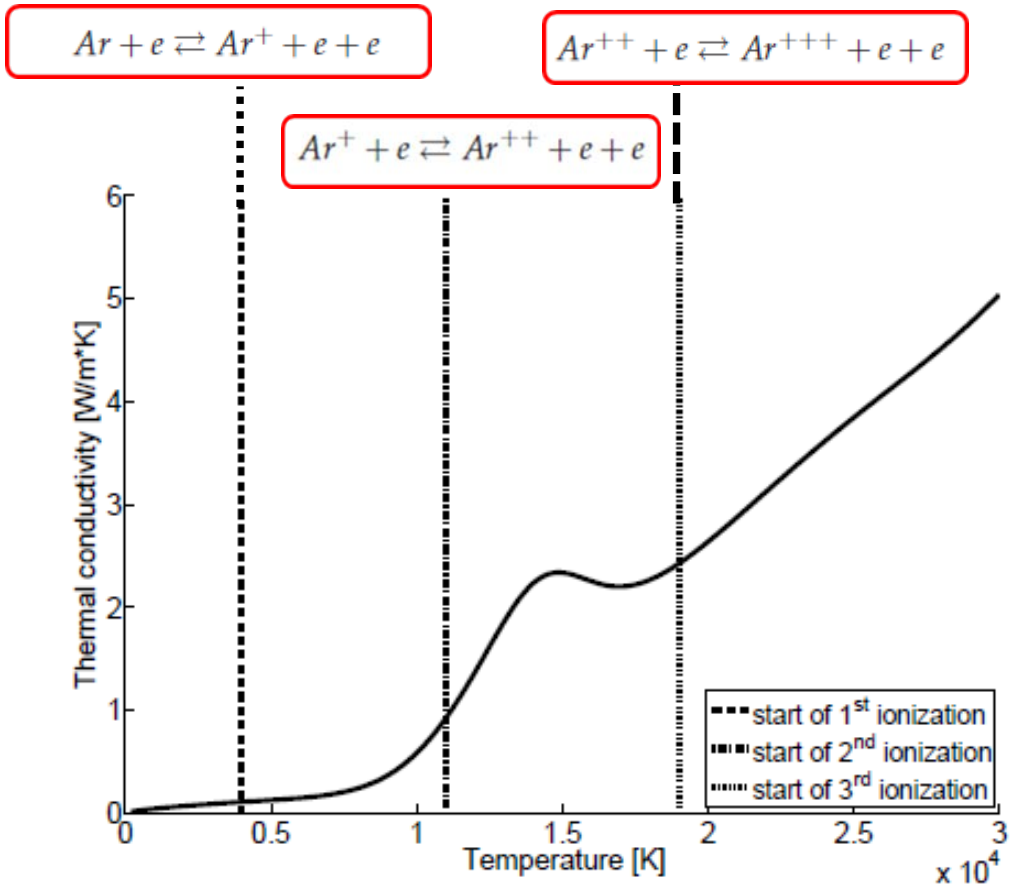


Figure 2.4: Thermal conductivity of an argon gas versus temperature.

From "Plasma arc welding simulation with openFOAM", M. Sass-Tisovskaya, Lic. thesis, Dept. Applied Mechanics, Chalmers University of Technology, 2009 (page 31)

Heat transfer and buoyancy-driven flows	
buoyantBoussinesqPimpleFoam	Transient solver for buoyant, turbulent flow of incompressible fluids
buoyantBoussinesqSimpleFoam	Steady-state solver for buoyant, turbulent flow of incompressible fluids
buoyantPimpleFoam	Transient solver for buoyant, turbulent flow of compressible fluids for ventilation and heat-transfer
buoyantSimpleFoam	Steady-state solver for buoyant, turbulent flow of compressible fluids
chtMultiRegionFoam	Combination of heatConductionFoam and buoyantFoam for conjugate heat transfer between a solid region and fluid region
chtMultiRegionSimpleFoam	Steady-state version of chtMultiRegionFoam
thermoFoam	Evolves the thermodynamics on a frozen flow field

OpenFOAM solver heatTransfer/thermoFoam: *(6/16)*

- **Copy the solver in your user directory and rename**:
  cd $WM_PROJECT_USER_DIR/applications/solvers/heatTransfer
  rk: if you do not yet have the heatTransfer directory under /solvers, create it (mkdir heatTransfer)
  cp -r $WM_PROJECT_DIR/applications/solvers/heatTransfer/thermoFoam .
  mv thermoFoam myThermoFoam
  cd myThermoFoam
  mv thermoFoam.C myThermoFoam.C

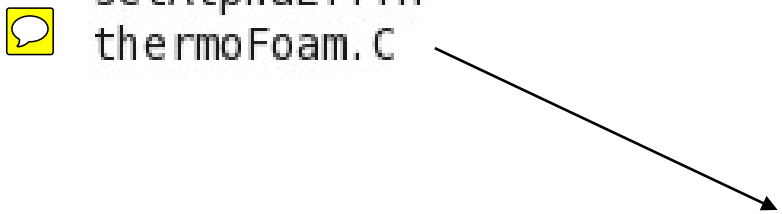
- **Modify Make/files to**
  myThermoFoam.C
  EXE = $(FOAM_USER_APPBIN)/myThermoFoam

- **Clean and compile**
  wclean
  wmake

OpenFOAM solver heatTransfer/thermoFoam: *(7/16)*

Parts of thermoFoam involving a thermophysical model

```
createFields.H
EEqn.H
Make
setAlphaEff.H
thermoFoam.C
```



```
...
#include "rhoThermo.H"
...
#include "EEqn.H"
...
```

Include a thermophysic library

Include an energy conservation equation

OpenFOAM solver heatTransfer/thermoFoam: (8/16)

Part of the energy conservation equation Eeqn.H

```
volScalarField& he = thermo.he();

fvScalarMatrix EEqn
(
    fvm::ddt(rho, he) + fvm::div(phi, he)
  + fvc::ddt(rho, K) + fvc::div(phi, K)
  + (
        he.name() == "e"
      ? fvc::div
        (
            fvc::absolute(phi/fvc::interpolate(rho), U),
            p,
            "div(phiv,p)"
        )
      : -dpdt
    )
  - fvm::laplacian(alphaEff, he)
 ==
    radiation->Sh(thermo)
  + fvOptions(rho, he)
);
```

"he" is either the specific internal energy or the specific enthapy (choice done when preparing a case, in the dictionnary constant/thermophysicalProperties)

Energy conservation -total energy of flowing fluid: $\rho\left(\hat{h}+K\right)$ - in a control volume moving at $\mathbf{v_b}$

$$\frac{d}{dt}\int_V \rho\left(\hat{h}+K\right)dV+\int_S \rho\left(\hat{h}+K\right)(\mathbf{v}-\mathbf{v_b})\cdot\mathbf{ds}-\frac{d}{dt}\int_V p dV-\int_S p(\mathbf{v}-\mathbf{v_b})\cdot\mathbf{ds}=-\int_S \mathbf{q}\cdot\mathbf{ds}-\int_S (p\mathbf{v}+\boldsymbol{\tau}\cdot\mathbf{v})\cdot\mathbf{ds}$$

Enthalpy : $\hat{h}=\hat{e}+\frac{p}{\rho}$

specific enthapy $\hat{h}$ or specific internal energy $\hat{e}$

Kinetic energy: *K*

```
  fvm::ddt(rho, he) + fvm::div(phi, he)
+ fvc::ddt(rho, K) + fvc::div(phi, K)
+ (
      he.name() == "e"
    ? fvc::div
      (
          fvc::absolute(phi/fvc::interpolate(rho), U),
          p,
          "div(phiv,p)"
      )
    : -dpdt
  )
- fvm::laplacian(alphaEff, he)
```

Energy conservation -total energy of flowing fluid: $\rho\left(\hat{h}+K\right)$ - in a control volume moving at $\mathbf{v_b}$

$$\frac{d}{dt}\int_V \rho\left(\hat{h}+K\right)dV+\int_S \rho\left(\hat{h}+K\right)(\mathbf{v}-\mathbf{v_b})\cdot\mathbf{ds}-\frac{d}{dt}\int_V p dV-\int_S p(\mathbf{v}-\mathbf{v_b})\cdot\mathbf{ds}=-\int_S \mathbf{q}\cdot\mathbf{ds}-\int_S (p\mathbf{v}+\boldsymbol{\tau}\cdot\mathbf{v})\cdot\mathbf{ds}$$

specific kinetic energy K

```
    fvm::ddt(rho, he) + fvm::div(phi, he)
  + fvc::ddt(rho, K) + fvc::div(phi, K)
  + (
        he.name() == "e"
      ? fvc::div
        (
            fvc::absolute(phi/fvc::interpolate(rho), U),
            p,
            "div(phiv,p)"
        )
      : -dpdt
    )
  - fvm::laplacian(alphaEff, he)
```

Energy conservation -total energy of flowing fluid: $\rho\left(\hat{h}+K\right)$ - in a control volume moving at $\mathbf{v_b}$ *(11/16)*

$$\frac{d}{dt}\int_V \rho\left(\hat{h}+K\right)dV+\int_S \rho\left(\hat{h}+K\right)(\mathbf{v}-\mathbf{v_b})\cdot\mathbf{ds}-\frac{d}{dt}\int_V pdV-\int_S p(\mathbf{v}-\mathbf{v_b})\cdot\mathbf{ds}=-\int_S \mathbf{q}\cdot\mathbf{ds}-\int_S (p\mathbf{v}+\boldsymbol{\tau}\cdot\mathbf{v})\cdot\mathbf{ds}$$

```
  fvm::ddt(rho, he) + fvm::div(phi, he)
+ fvc::ddt(rho, K) + fvc::div(phi, K)
+ (
    he.name() == "e"
      ? fvc::div
        (
            fvc::absolute(phi/fvc::interpolate(rho), U),
            p,
            "div(phiv,p)"
        )
      : -dpdt
  )
- fvm::laplacian(alphaEff, he)
```

If "he" is the specific enthalpy "$\hat{h}$" → *This is not true (as he is not "e")*

so this part is not used

while this term is calculated

Energy conservation -total energy of flowing fluid: $\rho(\hat{h}+K)$ - in a control volume moving at $\mathbf{v_b}$ *(12/16)*

$$\frac{d}{dt}\int_V \rho\left(\hat{h}+K\right)dV+\int_S \rho\left(\hat{h}+K\right)(\mathbf{v}-\mathbf{v_b})\cdot\mathbf{ds}-\frac{d}{dt}\int_V pdV-\int_S p(\mathbf{v}-\mathbf{v_b})\cdot\mathbf{ds}=-\int_S \mathbf{q}\cdot\mathbf{ds}-\int_S (p\mathbf{v}+\boldsymbol{\tau}\cdot\mathbf{v})\cdot\mathbf{ds}$$

$$\hat{h}=\hat{e}+\frac{p}{\rho}$$

If "he" is the specific internal energy $\hat{e}$

```
    fvm::ddt(rho, he) + fvm::div(phi, he)
  + fvc::ddt(rho, K) + fvc::div(phi, K)
  + (
      he.name() == "e"
        ? fvc::div
          (
              fvc::absolute(phi/fvc::interpolate(rho), U),
              p,
              "div(phiv,p)"
          )
        : -dpdt
    )
  - fvm::laplacian(alphaEff, he)
```

This is true

so this term is calculated

while this part is not used

Energy conservation -total energy of flowing fluid: $\rho(\hat{h}+K)$ - in a control volume moving at $\mathbf{v_b}$ *(13/16)*

$$\frac{d}{dt}\int_V \rho\left(\hat{h}+K\right)dV+\int_S \rho\left(\hat{h}+K\right)(\mathbf{v}-\mathbf{v_b})\cdot\mathbf{ds}-\frac{d}{dt}\int_V pdV-\int_S p(\mathbf{v}-\mathbf{v_b})\cdot\mathbf{ds}=-\int_S \mathbf{q}\cdot\mathbf{ds}+\int_S (p\mathbf{v}+\boldsymbol{\tau}\cdot\mathbf{v})\cdot\mathbf{ds}$$

$$\hat{h}=\hat{e}+\frac{p}{\rho}$$

```
  fvm::ddt(rho, he) + fvm::div(phi, he)
+ fvc::ddt(rho, K) + fvc::div(phi, K)
+ (
      he.name() == "e"
    ? fvc::div
      (
          fvc::absolute(phi/fvc::interpolate(rho), U),
          p,
          "div(phiv,p)"
      )
    : -dpdt
  )
- fvm::laplacian(alphaEff, he)
```

conduction heat flux

alphaEff (the thermal diffusivity) is made of 2 contributions:

alphaEff = **alpha laminar** + *alpha turbulent*

It is set in solver/heatTransfer/thermoFoam/setAlphaEff.H

via the turbulence library : src/turbulenceModels `turbulence->alphaEff();`

the ”turbulenceModels” library is linked to the thermo library src/thermophysicalModels

so if the executables are renamed in a new thermophysical library and the library is compiled, they need to be renamed when they appear in the Make/options of the turbulenceModels library and the turbulenceModels library needs also to be compiled (in $WM_PROJECT_USER_DIR)

alpha turbulent is defined in *src/turbulenceModels*

alpha laminar is defined in **src/thermophysicalModels** (as transport property)

What do we need to implement ?

In EEqn.H the heat flux is writen : $q = -$ alphaEff ∇he

where the laminar part of alphaEff is either:

κ / C_p if *"he"* represents the specific enthalpy *h* *(we will work with this case and from now assume he=h)*

or

κ / C_v if *"he"* represents the specific internal energy *e*

So we **need to implement the thermal conductivity** $\kappa = \kappa(T)$ - *plotted slide 16 (right).*
the **density, and the specific heat capacity,** *respectively plotted slide 15 and 16*, so that $C_p = \rho(T).c_p(T)$.

But this is not sufficient since the conservative variable in EEqn.H is the specific enthalpy *h*
while the termodynamic and transport properties depend on another variable: the temperature *T*.
So we also need to determine *T* from *h*. This is done solving (with an iterative procedure already implemented in OpenFAOM) the equation of state

$$\Delta h = \int_{T_{ref}}^{T} c_p(T)\, dT$$

It implies that we **also need to implement the specific enthalpy** *h = h(T).*

This implementation can be done in 2 parts

1. First, the implementation of the new transport property κ (the thermal conductivity) for a temperature range from 200K to 20kK. It will be implemented, compiled and tested.

   Rk. The resultant thermophysical model will not be consistent from a physical point of view (as it will be associated with constant enthalpy, constant specific heat, …). But it runs and has the advantage of allowing splitting the implementation work in smaller parts (easier to debug).

2. Implement the new thermodynamic properties C_p and h and the new equation of state ρ.
   These must be implemented together to be able to derive the temperature T from *h(T)* using $c_p(T)$.

   Rk. The resultant thermophysical model will then be consistent from a physical point of view.
   It can be observed that the consitent model runs faster than the non-consistent model implemented in the 1st part.

Implement a new transport property K: main steps *(1/12)*

Step 0 : import and rename suited parts of the library ”thermophysicalModels”

Step 1 : declare the new transport property model (see Ic)*

Step 2 : define the new transport property model (see Ic)*

Step 3: declare the new thermophysical model (see III)**

Step 4 : link the new thermophysical model to the solver

Step 5 : call the new thermophysical model in a test case

**Slide 6* ** *Slide 7*

Implement a new transport property K: step 0 *(2/12)*

Prepare your library myThermophysicalModels/mySpecie

- **Copy the folder "specie" of the library in your user directory and rename it**:
  cd $WM_PROJECT_USER_DIR/src/myThermophysicalModels
  rk: if you do not yet have the directory myThermophysicalModels under /src, create it with mkdir
  cp -r $WM_PROJECT_DIR/src/thermophysicalModels/specie .
  mv specie mySpecie
  cd mySpecie

- **Modify the Make/files to:**
  mySpecie.C
  LIB = $(**FOAM_USER_LIBBIN**)/libspecie

- **Clean & compile**
  wclean
  wmake libso

Now the executable is in your working space, and your "libspecie" will be accessed in priority (instead of the OpenFOAM executable in $FOAM_LIBBIN, even if the name is the same)

Then this name of executable can be kept unchanged. Doing so, no need to import the turbulence library, no need to rename its links (in Make/options) to your thermo library, and no need to recompile the turbulence library (See slide 28):
the $FOAM_LIBBIN turbulence library will link to your own thermo library.

Implement a new transport property K: step 0 *(3/12)*

Prepare your library myThermophysicalModels/myBasic

- **Copy the folder "basic" of the library in your user directory and rename it**:

```
cd $WM_PROJECT_USER_DIR/src/myThermophysicalModels
cp  -r  $WM_PROJECT_DIR/src/thermophysicalModels/basic .
mv basic myBasic
cd myBasic
```

- **Modify Make/files to:**

myBasic.C

LIB = $(**FOAM_USER_LIBBIN**)/libfluidThermophysicalModels

Similar to the previous slide

Implement a new transport property K: step 0 *(4/12)*

- **Modify the Make/options file to** *(since myBasic needs to be linked to mySpecie at compilation)*

```
EXE_INC = \
    -I$(LIB_SRC)/finiteVolume/lnInclude \
    -I$(WM_PROJECT_USER_DIR)/src/myThermophysicalModels/mySpecie/lnInclude \
    -I$(LIB_SRC)/meshTools/lnInclude


LIB_LIBS = \
    -L$(FOAM_USER_LIBBIN) \
    -lfiniteVolume \
    -lspecie
```

(1) Gives the path to access your own files located in mySpecie

(2) Indicates that the compilator must 1st look in your own working space (in $FOAM_USER_LIBBIN) to pick the libraries listed below. If not found there (ex. may be lfiniteVolume is not in your space $FOAM_USER_LIBBIN) the compilator will next look in the OpenFOAM space (in $FOAM_LIBBIN).
If still not found it will complain.

- **Clean the dependencies and compile**

```
wclean
wmake libso
```

(3) Can check the path used by reading the messages writen on the screen during compilation (see next slide)

How to check that the compiler links the desired libraries ?

```
[isabelle@cluster myBasic]$ wclean
[isabelle@cluster myBasic]$ wmake libso
wmakeLnInclude: linking include files to ./lnInclude
Making dependency list for source file basicThermo/basicThermo.C
Making dependency list for source file fluidThermo/fluidThermo.C
Making dependency list for source file psiThermo/psiThermo.C
Making dependency list for source file psiThermo/psiThermos.C
Making dependency list for source file rhoThermo/rhoThermo.C
Making dependency list for source file rhoThermo/rhoThermos.C
Making dependency list for source file derivedFvPatchFields/fixedEnergy/fixedEnergyFvPatchScalarField.C
Making dependency list for source file derivedFvPatchFields/gradientEnergy/gradientEnergyFvPatchScalarF
ield.C
Making dependency list for source file derivedFvPatchFields/mixedEnergy/mixedEnergyFvPatchScalarField.C
Making dependency list for source file derivedFvPatchFields/energyJump/energyJump/energyJumpFvPatchScal
arField.C
Making dependency list for source file derivedFvPatchFields/energyJump/energyJumpAMI/energyJumpAMIFvPat
chScalarField.C
SOURCE=basicThermo/basicThermo.C ;  g++ -m64 -Dlinux64 -DWM_DP -Wall -Wextra -Wno-unused-parameter -Wol
d-style-cast -Wnon-virtual-dtor -O3  -DNoRepository -ftemplate-depth-100 -I/home/isabelle/OpenFOAM/Open
FOAM-2.3.x/src/finiteVolume/lnInclude -I/home/isabelle/OpenFOAM/isabelle-2.3.x/src/myThermophysicalMode
ls/mySpecie/lnInclude -I/home/isabelle/OpenFOAM/OpenFOAM-2.3.x/src/meshTools/lnInclude -IlnInclude -I.
-I/home/isabelle/OpenFOAM/OpenFOAM-2.3.x/src/OpenFOAM/lnInclude -I/home/isabelle/OpenFOAM/OpenFOAM-2.3.
x/src/OSspecific/POSIX/lnInclude   -fPIC -c $SOURCE -o Make/linux64GccDPOpt/basicThermo.o
SOURCE=fluidThermo/fluidThermo.C ;  g++ -m64 -Dlinux64 -DWM_DP -Wall -Wextra -Wno-unused-parameter -Wol
d-style-cast -Wnon-virtual-dtor -O3  -DNoRepository -ftemplate-depth-100 -I/home/isabelle/OpenFOAM/Open
FOAM-2.3.x/src/finiteVolume/lnInclude -I/home/isabelle/OpenFOAM/isabelle-2.3.x/src/myThermophysicalMode
ls/mySpecie/lnInclude -I/home/isabelle/OpenFOAM/OpenFOAM-2.3.x/src/meshTools/lnInclude -IlnInclude -I.
-I/home/isabelle/OpenFOAM/OpenFOAM-2.3.x/src/OpenFOAM/lnInclude -I/home/isabelle/OpenFOAM/OpenFOAM-2.3.
x/src/OSspecific/POSIX/lnInclude   -fPIC -c $SOURCE -o Make/linux64GccDPOpt/fluidThermo.o
SOURCE=psiThermo/psiThermo.C ;  g++ -m64 -Dlinux64 -DWM_DP -Wall -Wextra -Wno-unused-parameter -Wold-st
yle-cast -Wnon-virtual-dtor -O3  -DNoRepository -ftemplate-depth-100 -I/home/isabelle/OpenFOAM/OpenFOAM
-2.3.x/src/finiteVolume/lnInclude -I/home/isabelle/OpenFOAM/isabelle-2.3.x/src/myThermophysicalModels/m
ySpecie/lnInclude -I/home/isabelle/OpenFOAM/OpenFOAM-2.3.x/src/meshTools/lnInclude -IlnInclude -I. -I/h
```

…

*Here it can be checked that the library "finiteVolume" is picked in /home/…/**OpenFOAM2.3.x**/src (so in $WM_PROJECT_DIR/src) since it does not exist in $WM_PROJECT_USER_DIR/src*

Same for meshTools

*There it can be checked that "myThermophysicalModels/mySpecie" is picked in /home/…/**isabelle-2.3.x**/src (so in $WM_PROJECT_USER_DIR/src) and not in $WM_PROJECT_DIR*

Implement a new transport property K: step 1 *(6/12)*

Declare the new transport model in user src/myThermophysicalModels/mySpecie

- **In mySpecie/include/thermoPhysicsTypes.H add the following lines**

```
#include "kineticArTransport.H"

typedef
kineticArTransport
<
    species::thermo
    <
        hConstThermo
        <
            perfectGas<specie>
        >,
        sensibleEnthalpy
    >
> kineticArGasHThermoPhysics;
```

To access the new transport model

Name given to the new transport model

Name given to the new thermophysical model

Implement a new transport property K: step 2 *(7/12)*

Define the new transport model in user src/myThermophysicalModels/mySpecie

- **Copy and rename an existing model:** *(Prepare the structure)*

  cd transport
  cp –r const kineticAr
  cd kineticAr
  mv constTransport.C kineticArTransport.C
  mv constTransport.H kineticArTransport.H
  mv constTransportI.H kinticArTransportI.H

  open the files one by one and replace
  "constTransport" (NOT just "const" !) with "kineticArTransport"

  update the "instantiated type name" in kineticArTransport.H

  so look for "instantiaded" and below (only there!) replace "return "const" " with " return "kineticAr" "

- **Clean the dependencies** ("wclean") **and compile mySpecie** ("wmake libso")

Implement a new transport property K: step 2 *(8/12)*

- **Open** kinticArTransportI.H

```
// Thermal condicivity changed from constant to tabulated data table
template<class Thermo>
inline Foam::scalar Foam::kineticArTransport<Thermo>::kappa
(
    const scalar p,
    const scalar T
) const
{
    // original version:
    //return this->Cpv(p, T)*mu(p, T)*rPr_;

  // new version for argon plasma:
  // Thermal conductivity kappa [W/(m.K)] function of T, for Argon plasma,
  // tabulated for T from T0=200K to 20000K
  // with tabulation interval of dT=100K

   int i_index;
   scalar dT=100;
   …
   return kappa_T_Argon;
 // end of kappa version implemented for argon plasma
```

thermal conductivity

Comment the original model

insert** the new model provided in **the file Ar_Data_ThermalConduct

Implement a new transport property K: step 2 *(9/12)*

```
// Thermal diffusivity for enthalpy [kg/ms]
//
template<class Thermo>
inline Foam::scalar Foam::kineticArTransport<Thermo>::alphah
(
    const scalar p,
    const scalar T
) const
{
    // original version (with Pr constant):
    //return mu(p, T)*rPr_;

    // new version for argon plasma (since Pr is not constant):
    // Pr = mu(p,T)*Cp(p,T)/kappa(p,T)
    // mu(p,T)/Pr = kappa(p,T)/Cp(p,T)
    return kappa(p,T)/this->Cpv(p,T);

   // end of alpha version implemented for argon plasma
}
```

Comment the original model

Write the new model

- **Clean the dependencies** (“wclean”) **and compile mySpecie** (“wmake libso”)

Implement a new transport property K: step 3 *(10/12)*

Declare the new thermophysical model in user src/myThermophysicalModels/myBasic

- **In myBasic/rhoThermo/rhoThermos.C add the following lines**

```
#include "kineticArTransport.H"
makeThermo
(
    rhoThermo,
    heRhoThermo,
    pureMixture,
    kineticArTransport,
    sensibleEnthalpy,
    hConstThermo,
    perfectGas,
    specie
);
```

New combination of Ia, Ib, Ic, II and III (see slides 3 to 7) defining a new thermophysical model

- **Clean the dependencies** (“wclean”) **and compile myBasic** (“wmake libso”)

Implement a new transport property K: step 4 *(11/12)*

Link the new thermophysicalModel library to the solver

- **In myThermoFoam/Make/options do the following changes to access the new library**

```
-I$(LIB_SRC)/thermophysicalModels/basic/lnInclude \
```



```
-I$(WM_PROJECT_USER_DIR)/src/myThermophysicalModels/myBasic/lnInclude \

EXE_LIBS = \
    -lfiniteVolume \
```



```
EXE_LIBS = \
    -L$(FOAM_USER_LIBBIN) \
    -lfiniteVolume \
```

- **Clean the dependencies** (wclean) **and compile myThermoFoam.C** (wmake)

Implement a new transport property K: step 5 *(12/12)*

Call the new thermophysicalModel in a test case

- **Use the test case provided: blockThermoFoamCase.tgz**
- **Run this case with the solver thermoFoam (the original one)**
- **Copy blockThermoFoam to blockNewThermoFoam and clean**
- **Update constant/thermophysicalPropersties to**

```
thermoType
{
    type            heRhoThermo;
    mixture         pureMixture;
    transport       kineticAr;   // new model
  //transport       const;
    thermo          hConst;
    equationOfState perfectGas;
    specie          specie;
    energy          sensibleEnthalpy;
}
```

- **Run this case with the solver myThermoFoam linked to the new thermophysical library**
- **Compare the results (for instance doing a plot along a suited line you can choose)**

This implementation can be done in 2 parts

1. First, the implementation of the new transport property κ (the thermal conductivity) for a temperature range from 200K to 20kK. It will be implemented, compiled and tested.

   Rk. The resultant thermophysical model will not be consistent from a physical point of view (as it will be associated with constant enthalpy, constant specific heat, …). But it runs and has the advantage of allowing splitting the implementation work in smaller parts (easier to debug).

2. Implement the new thermodynamic properties C_p and h and the new equation of state ρ.
   These must be implemented together since the aim is to be able to derive the temperature T from $h(T)$ and to calculate the heat capacity $C_p = \rho(T).c_p(T)$

   Rk. The resultant thermophysical model will then be consistent from a physical point of view.
   It can also be observed that the consitent model runs faster than the non-consistent model implemented in the 1st step

Part 1 is done. We now start this 2^{nd} part

Implement new thermodynamic properties and a new equation of state *(2/16)*

Step 1 : declare (see Ia, b) #,* the new thermodynamic properties and the new equation of state

Step 2 : define (see Ia) # the new equation of state

Step 3 : define (see Ib)* the new themodynamic properties

Step 4: declare (see III)** the new thermophysical model

Step 5 : link the new thermophysical model to the solver

Step 6 : call the new thermophysical model in a test case and run

#*See slide 4* **See slide 5* *** See slide 7*

Implement new thermodynamic properties and equation of state: step 1 *(3/16)*

Declare the new models in user src/myThermophysicalModels/mySpecie

- **In mySpecie/include/thermoPhysicsTypes.H add**

```
#include "hKineticArThermo.H"
#include "rhoKineticAr.H"
```

To access the new thermodynamic model & the new equation of state

and modify

```
typedef
kineticArTransport
<
    species::thermo
    <
        hConstThermo
        <
            perfectGas<specie>
        >,
        sensibleEnthalpy
    >
> kineticArGasHThermoPhysics;
```

Name given to the new thermodynamic model & equation of state

to

```
typedef
kineticArTransport
<
    species::thermo
    <
        hKineticArThermo
        <
            rhoKineticAr<specie>
        >,
        sensibleEnthalpy
    >
> kineticArGasHThermoPhysics;
```

Implement new thermodynamic properties and equation of state: step 2 *(4/16)*

Define a new equation of state in in user src/myThermophysicalModels/mySpecie

- **Copy and rename an existing model:**

Prepare the structure

cd equationOfState
cp –r perfectGas rhoKineticAr
cd rhoKineticAr
mv perfectGas.C rhoKineticAr.C
mv perfectGas.H rhoKineticAr.H
mv perfectGastI.H rhoKinticArI.H
open the files one by one and replace
"perfectGas" with "rhoKineticAr"

update the "instantiated type name" in rhoConstAr.H
so look for "instantiaded" and below replace "return "perfectGas<" "
with " return "rhoKineticAr<" "

Implement new thermodynamic properties and equation of state: step 2 *(5/16)*

- **Open** rhoKineticArI.H and do the following modifications:

density

```
template<class Specie>
inline Foam::scalar Foam::rhoKineticAr<Specie>::rho(scalar p, scalar T) const
{
    //old model
    //return p/(this->R()*T);

    //new model
    // Density [kg/m^3] function of T, for Argon plasma,
    // tabulated for T from T0=200K to 20000K
    // with tabulation interval of dT=100K

    int i_index;
    scalar dT=100;
    scalar T0=200;
    scalar Temp_Argon;
    scalar rho_T_Argon;

    ...
    return rho_T_Argon;
}
```

Comment the original model

insert** the new model provided in **the file density_Ar_Data

Implement new thermodynamic properties and equation of state: step 2 *(6/16)*

- **Modify also**

compressibility

```
template<class Specie>
inline Foam::scalar Foam::rhoKineticAr<Specie>::psi(scalar, scalar T) const
{
  // old model
  //return 1.0/(this->R()*T);

  //new model
    Info << " psi should not be used with the rhoKineticAr model " << endl;
    return 0.0;
}
```

Comment the original model (ideal gas)

Write the new model
Rk: psi is set to zero since the plasma model implemented here is mechanically incompressible, and thermaly expansible: $\rho(P,T) = \rho(T)$.

Implement new thermodynamic properties and equation of state: step 2 *(7/16)*

- **Modify also**

```
template<class Specie>
inline Foam::scalar Foam::rhoKineticAr<Specie>::Z(scalar, scalar) const
{
  // old model
  //return 1.0;

  //new model
    Info << " Z should not be used with the rhoKineticAr model " << endl;
    return 0.0;
}
```

Compressibility factor

Comment the original model (ideal gas)

Write the new model

Implement new thermodynamic properties and equation of state: step 2 *(8/16)*

- **Modify also**

```
template<class Specie>
inline Foam::scalar Foam::rhoKineticAr<Specie>::cpMcv(scalar, scalar) const
{
  // old model
  //return this->RR;

  //new model
    Info << " cpMcv should not be used with the rhoKineticAr model " << endl;
    return 0.0;
}
```

Comment the original model

write the new model

- **Clean and compile mySpecie**

  wclean

  wmake libso

Implement new thermodynamic properties and equation of state: step 3 *(9/16)*

Define the new properties h, C_p in user src/myThermophysicalModels/mySpecie

- **Copy and rename an existing model:** *Prepare the structure*

cd thermo
cp –r hConst hKineticAr
cd hKineticAr
mv hConstThermo.C hKineticArThermo.C
mv hConstThermo.H hKineticArThermo.H
mv hConstThermoI.H hKinticArThermoI.H

open the files one by one and replace
"hConstThermo" with "hKineticArThermo"

update the "instantiated type name" in hKineticArThermo.H
so look for "instantiaded" and below replace "return "hConst<" "
with " return "hKineticAr<" "

Implement new thermodynamic properties and equation of state: step 2 *(10/16)*

- **Open hKineticArI.H and do the following modifications:**

```
template<class equationOfState>
inline Foam::scalar Foam::hKineticArThermo<equationOfState>::cp
(
    const scalar p,
    const scalar T
) const
{
    // original model
    //return Cp_;

    // New model:
    // heat capacity at constant pressure [J/(kmol.K)] function of T,
    // for Argon plasma,
    // tabulated for T from T0=200K to 20000K
    // with tabulation interval of dT=100K

    int i_index;
    scalar dT=100;
    ...
    return Cp_T_Argon*this->W();

    // end of cp version implemented for argon plasma
}
```

Heat capacity at constant pressure

Comment the original model

insert** the new model provided in **the file heatCapacity_Cp_Data

Implement new thermodynamic properties and equation of state: step 3 *(11/16)*

- **Modify also**

```
template<class equationOfState>
inline Foam::scalar Foam::hKineticArThermo<equationOfState>::ha
(
    const scalar p, const scalar T
) const
{
    // original model
    //return Cp_*T + Hf_;

    // enthalpy [J/kg] function of T, for Argon plasma,
    // tabulated for T from T0=200K to 20000K
    // with tabulation interval of dT=100K

    int i_index;
    scalar dT=100;
    ...
    return h_T_Argon*this->W();

  // end of h version implemented for argon plasma

}
```

absolute enthalpy
Hf is the enthalpy of formation

Comment the original model

insert** the new model provided in **the file enthalpy_Data.
Rk. The reference temperature was set so that Hf is zero.

Implement new thermodynamic properties and equation of state: step 3 *(12/16)*

- **Modify also**

```
template<class equationOfState>
inline Foam::scalar Foam::hKineticArThermo<equationOfState>::hs
(
    const scalar p, const scalar T
) const
{
    // original model
    //return Cp_*T;

    return ha(p,T)-hc();
}
```

sensible enthalpy

Comment the original constant model

Write the new temperature dependent model.
Rk. As the non constant thermodynamic models in openFoam depend on both pressure p and temperature, we write ha(p,T) although p is not used.

Implement new thermodynamic properties and equation of state: step 3 *(13/16)*

- **Modify also**

```
template<class equationOfState>
inline Foam::scalar Foam::hKineticArThermo<equationOfState>::hc() const
{
    // original model
    //return Hf_;

    return 0.;
}
```

chemical enthalpy

Comment the original model

Write the new model

Rk. Here the plasma is considered as one-fluid. The ionization reactions were accounted for when tabulating the absolute enthalpy ha. For a one-fluid model hc is the enthalpy of formation. Here it is set to zero (see the remark on slide 53).

- **Clean (wclean) and compile mySpecie (wmake libso)**

Implement new thermodynamic properties and equation of state: step 4 *(14/16)*

Declare the new thermophysical model in user src/myThermophysicalModels/myBasic

- **In myBasic/rhoThermo/rhoThermos.C add the following lines**

```
#include "hKineticArThermo.H"
#include "rhoKineticAr.H"
```

→ *To access the new thermodynamic model & the new equation of state*

and change

```
makeThermo
(
    rhoThermo,
    heRhoThermo,
    pureMixture,
    kineticArTransport,
    sensibleEnthalpy,
    hConstThermo,
    perfectGas,
    specie
);
```

Name given to the new thermodynamic model & equation of state

to:

```
makeThermo
(
    rhoThermo,
    heRhoThermo,
    pureMixture,
    kineticArTransport,
    sensibleEnthalpy,
    hKineticArThermo,
    rhoKineticAr,
    specie
);
```

- **Clean (wclean) and compile myBasic (wmake libso)**

Implement new thermodynamic properties and equation of state: step 5 *(15/16)*

Link the new thermophysical model to the solver

- **The update of myThermoFoam/Make/options**
  needed to access the new thermophysical library
  has already been done when implementing the thermal conductivity κ (see slide 41)

  So nothing else needs to be done here (unless you decided to rename myBasic in part 2;
  in that case see slide 41).

Implement new thermodynamic properties and equation of state: step 6 *(16/16)*

Call the new thermophysical model in a test case and run

- **Copy blockThermoFoam to blockKineticArThermoFoam and clean (wclean)**
- **Update constant/thermophysicalPropersties to**

```
thermoType
{
    type            heRhoThermo;
    mixture         pureMixture;
    transport       kineticAr;    // new model
  //transport       const;
    thermo          hKineticAr;   // new model
  //thermo          hConst;
    equationOfState rhoKineticAr;  // new model
  //equationOfState perfectGas;
    specie          specie;
    energy          sensibleEnthalpy;
}
```

- **Run this case with the solver MyThermoFoam (now linked to your new thermophysical library)**
- **Compare the results with the previous results (doing a plot along a suited line you can choose)**