

The interfacial Temperature in reactingEulerFoam

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The interfacial temperature, T_f , is updated in
phaseSystems/PhaseSystems/InterfaceCompositionPhaseChangePhaseSystem
by the member function *correctThermo()*:

```
Tf -=
(
    H1*(Tf - pair.phase1().thermo().T())
    + H2*(Tf - pair.phase2().thermo().T())
    + mDotL
)
/(
    max(H1 + H2 + mDotLPrime, HSmall)
);
```

applying one step of the Newton's method ($T_f^{n+1} = T_f^n - \frac{G(T_f^n)}{G'(T_f^n)}$).

The equation $G(T_f)$ to be solved to find T_f is:

$$H_1(T_1 - T_f) + H_2(T_2 - T_f) = m\dot{L} \quad (1)$$

where H_1 and H_2 are defined in the same file with

```
volScalarField H1(this->heatTransferModels_[pair][pair.first()]->K());
volScalarField H2(this->heatTransferModels_[pair][pair.second()]->K());
```

The term $m\dot{L}$ and its derivative with respect to T_f ($m\dot{L}Prime$) are calculated before the Newton's step:

```
// Add latent heats from forward and backward models
if (this->interfaceCompositionModels_.found(key12))
{
    this->interfaceCompositionModels_[key12]->addMDotL
    (
        this->massTransferModels_[pair][pair.first()]->K(),
        Tf,
        mDotL,
        mDotLPrime
    );
}
if (this->interfaceCompositionModels_.found(key21))
{
    this->interfaceCompositionModels_[key21]->addMDotL
    (
        this->massTransferModels_[pair][pair.second()]->K(),
        Tf,
        mDotL,
        mDotLPrime
    );
}
```

The function *addMDotL* is defined in

```
/interfacialCompositionModels/interfaceCompositionModels/  
interfaceCompositionModel/interfaceCompositionModel.C
```

as a function of K , T_f , $mDotL$ e $mDotLPrime$:

```
forAllConstIter(hashedList, this->speciesNames_, iter)  
{  
    volScalarField rhoKDL  
    (  
thermo_.rhoThermo::rho()  
*K  
*D(*iter)  
*L(*iter, Tf)  
);  
  
mDotL += rhoKDL*dY(*iter, Tf);  
mDotLPrime += rhoKDL*YfPrime(*iter, Tf);  
}
```

where D is the mass diffusivity [m^2s^{-1}] and L is the specific latent heat [m^2s^{-2}].

$$D = \frac{\alpha_{ph}(p, T)}{\rho(p, T)} \frac{1}{Le}; \quad L = \Delta H_a. \quad (2)$$

In Eqs. (2) α_{ph}/ρ is the thermal diffusivity [m^2s^{-1}], Le is the Lewis dimensionless number defined as the ratio of thermal diffusivity to mass diffusivity and $H_a(p, T_f)$ is the specific enthalpy (to check better).

The equations solved for T_f is derived from a heat balance between the heat transferred between the liquid phase and the interface and the heat transferred between the gas phase and the interface:

$$Q_1 = H_1(T_f - T_1) - mDot \cdot Ha_1(T_f), \quad Q_2 = H_2(T_f - T_2) - mDot \cdot Ha_2(T_f). \quad (3)$$

Because neither heat nor mass can be stored on the phase interface, the overall heat balance must be satisfied

$$Q_1 + Q_2 = 0 \Rightarrow H_1(T_f - T_1) - mDot \cdot Ha_1(T_f) = H_2(T_f - T_2) - mDot \cdot Ha_2(T_f) \quad (4)$$

Rearranging the terms we obtain

$$H_1(T_1 - T_f) + H_2(T_2 - T_f) = mDot(Ha_2 - Ha_1) \quad (5)$$

and finally, substituting $L = (Ha_2 - Ha_1)$, we obtain Eq. (1).