The interfacial Temperature in reactingEulerFoam

 $March\ 15,\ 2017$

```
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.
   The equation to be solved to find T_f is:
                  H_1(T_1 - T_f) + H_2(T_2 - T_f) = mdotL
                                                                    (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 mdotL and its derivative with respect to T_f (mdotLPrime) 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(),
        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

/interfacial Composition Models/interface Composition Models/interface Composition Model/interface Composition Model. C

```
as a function of K, T_f, mDotL e mDotLPrime:
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```
forAllConstIter(hashedWordList, 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 $[m^2s^{-2}]$.

$$D = \frac{alphah(p,T)}{\rho(p,T)} \frac{1}{Le}; \qquad L = \Delta H_a$$
 (2)

where $alphah/\rho$ is the thermal diffusivity $[m^2s^{-1}]$, Le is the Lewis dimensionless number defined as the ratio of thermal diffusivity to mass diffusivity and $H_a(p,Tf)$ 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:

$$Q_1 = H1(T_f - T_1) - mDot \cdot Ha1(T_f) \qquad Q_2 = H2(T_f - T_2) - mDot \cdot Ha2(T_f)$$
(3)

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

$$Q_1+Q_2=0 \Rightarrow H1(T_f-T_1)-mDot\cdot Ha1(T_f)=H2(T_f-T_2)-mDot\cdot Ha2(T_f) \eqno(4)$$

Rearraging the terms we obtain

$$H1(T_1 - T_f) + H_2(T_2 - T_f) = mDot(Ha2 - Ha1)$$
(5)

and finally, substituting L = (Ha2 - Ha1), we obtain eq. 1.