

On the mathematical model simplification using constant Lewis number – Impact assessment on heterogeneous char conversion process

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Abstract

Reactive systems in a thermochemical conversion domain are modelled considering N-specie, 1-energy and 2-mass conservation equations assuming negligible pressure gradient resulting in N+3 non-linear coupled PDE system with dependency on thermodynamic and transport properties. Typically, simplistic temperature-dependent polynomials are chosen for estimating thermal conductivity and specific heat, however, the estimation of mass diffusion coefficient ($\mathcal{D}_{i,mix}$) follows a complicated procedure involving kinetic theory culminating in Chapman-Enskog equation. This renders the solution computationally intensive. The complexity is simplified by assuming a constant Lewis (Le) number, a standard practice in the analytical solution for conventional reactive systems. In fixing Le, ($\mathcal{D}_{i,mix}$) is equated to thermal diffusivity (a ratio of thermodynamic properties) resulting in the specie and energy equation yielding a similar solution and collapse of N+3 system of simultaneous equations to 3 equations. The current article explores the validity and limitation of assuming constant Le in the simulation of char conversion process in air and steam. Results of char conversion are compared for fixed Le and D estimated with Chapman-Enskog expression. The analysis suggests that Le remains invariant only under a severely restricted set of conditions. Fixing Le influences, the conversion process either over-/under-predicting the conversion time scales and the product gas composition.

Introduction

Thermochemical conversion processes are numerically modelled by a set of non-linear coupled equations expressing the conservation of mass, specie, momentum and energy, and a thermody-

amic equation of state describing the gas behaviour. Typical numerical models for char conversion consist of ‘N’ specie conservation equations, 2 mass conservations equations (for solid and gas phase), 1 momentum and 1 energy equation. The ‘N+4’ system of equations, supplemented by boundary conditions and ‘N+4’ interface conditions, are to be solved simultaneously, and in process thermodynamic and transport properties are also to be estimated, rendering the overall system complex and computationally intensive.

Among the thermodynamic and transport properties, estimation of the mass diffusivity coefficient ($\mathcal{D}_{i,mix}$) involves a mathematically rigorous approach requiring solution to complex kinetic theory-based equations. A straightforward and widely practiced approach to estimate the mass/specie diffusivity coefficient is deriving it from assumed Lewis number, first proposed by M. D. Smooke and V. Giovangigli [1], founding on methane-air premixed and non-premixed flames. Lewis number, a ratio of specie thermal diffusivity of the specie mass diffusivity is expressed as,

$$Le_i = \frac{\alpha}{\mathcal{D}_{i,mix}} = \frac{\lambda}{c_p \rho \mathcal{D}_{i,mix}} \Rightarrow \mathcal{D}_{i,mix} = \frac{\lambda}{c_p \rho Le_i} \quad (1)$$

assuming Le permits fixing $\mathcal{D}_{i,mix}$ with the knowledge of other thermodynamic properties i.e., λ , c_p , ρ ; which are relatively simpler to estimate using NASA polynomials[2]. A further simplification is invoked by assuming unity Lewis number. Treating all the species as being similar, $Le_i = Le = 1$, doing so implicitly signifies that the energy and specie conservation equations yield a similar solution (mathematically, the two equations are decoupled [3]), and hence implicitly, only 4 equation needs to be solved in place of ‘N + 4’ equation, like the Shvab-Zeldovich formulation [4].

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Unity/assumed Le introduces mathematical simplicity at the expense of underlying physics. In gaseous systems, species like H_2 and higher HC complexes have Le much different than unity. In heterogeneous system, especially in gas-solid reactions, an effective diffusivity and thereby an effective Le needs to be defined considering the porous characteristics and diffusion in pores.

In analyzing the system sensitivity to Le, it is observed that while the influence is nominal for homogeneous systems, it is profound for heterogeneous systems. In catalytic systems, the reaction zone's inability to adjust its position leads to super-adiabatic temperatures (adiabatic temperature derived for incoming mixture stoichiometry and temperature) under less than unity Le. This effect is more pronounced when the reactant (gaseous) is deficient (sub-stoichiometric), wherein the reactant specie is transported more efficiently to reacting surface than the heat away from it due to the prevailing gradients [5].

As such, it is argued that the influence of Le is significant in heterogeneous systems, particularly involving sub-stoichiometric reactions and systems with hydrogen as one of its constituents. It is important to note that, all the aforementioned features simultaneously prevail in a solid fuel gasification process, and assuming constant/unity Lewis number would potentially lead to significant error in model results.

In the current investigation, a one-dimensional model is used to evaluate the influence of Le on the thermochemical conversion (combustion/ gasification) of char in air, CO_2 and H_2O . The sensitivity of Lewis number investigated by comparing the model results obtained by use of Chapman-Enskog equation and Lennard-Jones coefficients for mass diffusivity with the model results arrived at by considering (a) unity Le for all species (b) constant non-unity Le for species.

Literature survey

In reviewing the literature, it is noted that the availability of literature accessing the impact of Lewis number on numerical models for large carbonaceous solid fuels is extremely limited.

J. C. M. Lee and D. Lauss[3], in their analytical and numerical investigations on the influence of Lewis number on heterogeneous catalysis, show that when Lewis number is less than unity, the

transient temperature exceeds the maximum possible temperature (adiabatic) under steady conditions, similar behaviour was experimentally observed by Hlavacek and Marek[6]. The analytical solution further showed that, for non-unity Lewis number the solution is not stable, not even asymptotically. The study concludes with a demonstration that internal temperature gradients in catalysts potentially yield large (≥ 1) Lewis numbers. However, since the analysis was based on Thiele modulus and effectiveness factor-based analysis, resolving intra-particle gradients was not possible.

Y. Uchida et al. and K. Kuwana et al. [7] investigates the influence of Lewis number on smouldering combustion of narrow solid fuels (thickness in the order of 100 microns). A series of parametric studies of oxidizer concentration, velocity and fuel type showed that Lewis number has a significant influence on the heterogeneous smouldering phenomena, thereby regarding it as one of the governing parameters. An effective Lewis number was defined considering the gas and solid phase's weighted thermal conductivity and taking the channel width (fuel thickness) into account. It was found that the effective Lewis number is of the order 0.1, a magnitude lower than unity Le. Similar studies have also been carried out by E.R. Ijioma et al.[8]

M. Nematollahi et al.[9] study the influence of Lewis number on coal pyrolysis and combustion. However, in all the cases considered, the coal particle diameter is less than 50 microns. This nullifies the diffusion of mass and energy within the particle and renders the case near homogeneous combustion. It is concluded that even under the near homogenized approach, the Lewis number is non-unity and varies between 0.4 – 1.4. Similarly, M. Bidabadi et al.[10] study the influence of Lewis number on pyrolysis and combustion of biomass dust and find the Lewis number to be non-unity.

It is evident from the review of the limited literature that the choice of specie diffusivity has a significant influence on the thermochemical conversion process, and the fact that efforts addressing the influence of Le in heterogeneous thermochemical conversions are extremely limited forms the basis for the current work.

Model formulation

The thermochemical conversion of a spherical char particle subjected to a reactive environment is modelled by application of mass, momentum and energy conservation equations with multi-step kinetics. The model developed is resolved in time and one-dimensional spherical space. The generalised formulation allows the model to solve for temperature and specie concentration within the particle. The resolution in space for the model developed allows establishing intra-particle gradients, which under limiting conditions can automatically act like shrinking core (impervious to reactant transport) or reacting core (reactant uniformity throughout) without any extraneous condition based intervention.

The processes occurring in char conversion process can be segregated into *condensed phase* involving intra-particle processes, and *gas phase* accounting for the homogeneous processes at the interface. A two-dimensional time freeze representation of a stationary spherical particle undergoing thermo-chemical conversion is presented in Figure 1.

Assumptions made

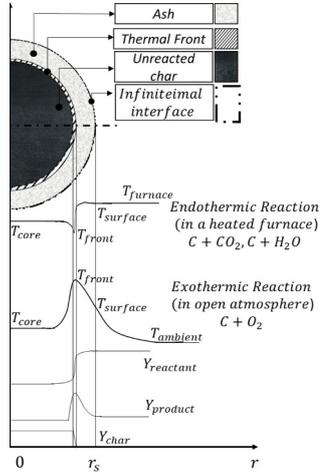


Figure 1: Single-particle conversion process - 2D time freeze representationl

- The conversion process is one dimensional
- Pressure gradient within the particle is neglected due to high porosity($\epsilon > 0.88$)[11].
- Gas and solid phase have uniform temperature.
- Infinitely thin, quasi-steady, non-reacting boundary layer

Condensed Phase

The phenomena in condensed phase can be described using unsteady species (Eq. 2) and energy conservation (Eq. 3) equations along with the continuity equations for solid phase (Eq. 4) and gas in the pores of the particle (Eq. 5),

$$\frac{\partial \rho_g \epsilon Y_i}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(-\rho_g v r^2 Y_i + r^2 \mathcal{D}_{i,eff} \rho_g \frac{\partial Y_i}{\partial r} \right) + \dot{\omega}_i''' \quad (2)$$

$$\frac{\partial \bar{\rho} \bar{c}_p T}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(-\bar{\rho} v r^2 \bar{c}_p T + r^2 \lambda_{eff} \frac{\partial T}{\partial r} \right) + H_c \dot{\omega}_c''' \quad (3)$$

$$\frac{\partial \epsilon}{\partial t} = \frac{-\dot{\omega}_c'''}{\rho_c} \quad (4)$$

$$\frac{\partial \rho_g \epsilon}{\partial t} = \frac{1}{r^2} \frac{-\rho_g v r^2}{\partial r} + \dot{\omega}_c''' \quad (5)$$

where $\bar{\rho} = (1 - \epsilon)\rho_c + \epsilon\rho_g$. In the above equations, ρ_c and ρ_g are the non-porous carbon and gas phase densities, weighted with particle porosity ϵ to obtain average particle density $\bar{\rho}$. In specie equation (2), Y_i represents the mass fraction of the species ($i = O_2, CO_2, CO, H_2, H_2O, CH_4$ and N_2) and T represents temperature in energy equation (3). The superficial velocity (v), in the convective terms of equations (2) and (3) is the apparent velocity with which the products are issuing out of the particle. The thermodynamic and transport properties (λ_{eff} , \bar{c}_p and $\mathcal{D}_{i,eff}$) are weighted average of the gas phase and solid phase properties. The volumetric reaction rate ($\dot{\omega}_i'''$) and the evolution of pore radius r_p (and surface area) are discussed further under the heading *chemical kinetics*.

The differential equation 2, 3 and 5 approach singularity at the particle core ($r \rightarrow 0$), to render the equations a conserved form, the independent coordinate r is transformed in terms of volume V .

$$V = \frac{4}{3} \pi r^3 \Rightarrow \frac{\partial}{\partial r} = 4\pi r^2 \frac{\partial}{\partial V} \quad (6)$$

$$\dot{m} = \rho_g A_{particle} v \Rightarrow \rho_g 4\pi r^2 v \Rightarrow \rho_g r^2 v = \frac{\dot{m}}{4\pi} \quad (7)$$

To obtain the mass flow rate (\dot{m}) of gasses issuing out of the particle, consistent with unsteady formulation, the equation of state $\rho_g = \frac{pM_g}{\mathcal{R}T}$ is ma-

nipulated to obtain,

$$\left[\frac{\rho_g \epsilon}{\bar{\rho}} \right] \frac{\partial \rho_g \epsilon}{\partial t} + \rho_g \left[1 - \frac{\rho_c \epsilon}{\bar{\rho}} \right] \frac{\partial \epsilon}{\partial t} - M_g \sum \frac{1}{M_i} \frac{\partial \rho_g \epsilon Y_i}{\partial t} - \left[\frac{\rho_g \epsilon}{\bar{\rho} \bar{c}_p T} \right] \frac{\partial \bar{\rho} \bar{c}_p T}{\partial t} = 0 \quad (8)$$

all the derivatives with respect to time in equation (8) are replaced using equations (2), (3), (4) and (5).

Gas Phase

The quasi-steady non reacting interface layer can be modelled by the following governing equations for specie and energy,

$$\frac{\dot{m}}{4\pi r^2} \frac{\partial Y_i}{\partial r} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\mathcal{D}_{i,mix} \rho_g r^2 \frac{\partial Y_i}{\partial r} \right) \quad (9)$$

$$\frac{\dot{m} c_{p,g}}{4\pi r^2} \frac{\partial T}{\partial r} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\lambda_g r^2 \frac{\partial T}{\partial r} \right) \quad (10)$$

The solution of interfacial equations (9) and (10) gives fluxes of species (11) and energy (12) across the interface,

$$\mathcal{D}_{i,mix} \rho_g \frac{\partial Y_i}{\partial r} = Q (Y_{i,\infty} - Y_{i,s}) \quad (11)$$

$$\lambda_g \frac{\partial T}{\partial r} = c_{p,g} Q (T_\infty - T_s) \quad (12)$$

$$Q = \frac{\dot{m}}{4\pi r_s^2} \frac{\exp(B_0)}{1 - \exp(-B_0)}; \quad B_0 = \frac{\dot{m} c_{p,g}}{4\pi r_s \lambda_g Nu}$$

In obtaining the above solution (11 and 12), empirical formulation for forced and free convection for heated spheres is considered from works of Dasappa et. al. [11].

Initial, Interface and Boundary conditions

The initial conditions (at $t = 0$) correspond to the set values of temperature and specie concentrations.

The interface conditions at $r = r_s$ are the continuity of fluxes,

$$\mathcal{D}_{i,mix} \rho_g \frac{\partial Y_i}{\partial r} = \lambda_g \frac{\partial T}{\partial r} = 0 \quad (13)$$

in equation (13), the expression for $\mathcal{D}_{i,mix} \rho_g \frac{\partial Y_i}{\partial r}$ and $\lambda_g \frac{\partial T}{\partial r}$ are obtained from interface equations (11) and (12).

The boundary conditions,

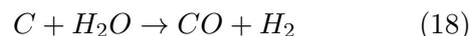
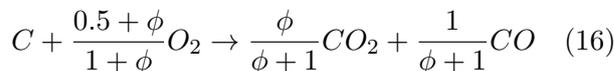
$$at \quad r = 0, \quad \frac{\partial T}{\partial V} = \frac{\partial Y_i}{\partial V} = 0 \quad (14)$$

$$as \quad r \rightarrow \infty, \quad T \rightarrow T_\infty, \quad Y_i \rightarrow Y_\infty \quad (15)$$

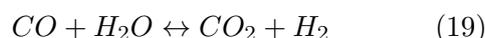
Chemical Kinetics

The heterogeneous (16-18) and homogeneous (19) reactions considered are described below, the rate constants and parameters are consolidated in table 1.

The heterogeneous reactions,



The homogeneous reaction,



The reaction of carbon with oxygen (Eq. 16) is adapted from Welsh et. al.[12].

$$\dot{\omega}_{C+O_2}'' = - \frac{M_c S_1 S_2 X_{OS}}{S_1 X_{OS} + S_2}; \quad (20)$$

Heterogeneous reaction rate of $C + CO_2$ reaction is chosen from works of J. Blackwood and A. Ingeme[13] and the reaction rate for $C + H_2O$ reaction is chosen from the studies of J. Blackwood and F. McGrory [14].

$$\dot{\omega}_{C+CO_2}'' = - \frac{k_1 p_{CO_2} - K_2 p_{CO}^2}{1 + K_3 p_{CO} + K_4 p_{CO_2}}; \quad (21)$$

$$\dot{\omega}_{C+H_2O}'' = - \frac{k_1 p_{H_2O} + K_4 p_{H_2} p_{H_2O} + K_5 p_{H_2O}^2}{1 + K_2 p_{H_2} + K_3 p_{H_2O}} \quad (22)$$

The reaction rate per unit area, $\dot{\omega}_i''$ are related to volumetric reaction rates, $\dot{\omega}_i'''$ by consideration of the diffusion processes, and modelled as enunciated in [15].

$$\dot{\omega}_C'' = \dot{\omega}_{C+O_2}'' + \dot{\omega}_{C+CO_2}'' + \dot{\omega}_{C+H_2O}'' \quad (23)$$

$$\dot{\omega}_C''' = \frac{\dot{\omega}_C'' S_g}{S_{g0}} = \frac{2\epsilon}{r_p} \quad (24)$$

S_g is the surface area per unit volume of the particle, approximated in terms of porosity and pore radius. The evolution of pore size can be modelled by considering the pores as long tubes (parallel pore model),

$$\rho_c \frac{\partial r_p}{\partial t} = \dot{\omega}_C'' \quad (25)$$

Table 1: Choice of Parameters

Property	Correlation/Value
ρ_c ($kg\ m^{-3}$)	1900
r_p ($t=0$) (μm)	50
λ_g ($W\ m^{-1}\ K^{-1}$)	Nasa Polynomial
μ_g ($Pa\ s$)	Nasa Polynomial
c_g ($kJ\ kg^{-1}\ K^{-1}$)	Nasa Polynomial
$\mathcal{D}_{i,mix}$ ($m^2\ s^{-1}$)	Stefan–Maxwell diffusion theory with Lennard-Jones potentials

Solution methodology

The solution requires integration of the parabolic system of partial differential equations (Eq.2-5) subjected to initial, interface and boundary conditions (Eq. 13-15), along with supplementary relations (Eq. 20-25). The system of equations are integrated using the Crank-Nicolson method. The method considers backward difference (implicit) for the time derivative and central difference approximation for space derivative.

The two grids, spatial and temporal are analysed for grid convergence, shown in Figure 3. A converging solution is obtained for a temporal step of 0.1 s or lower, and a spatial convergence is achieved for a grid size of 20 and above.

Model validation

The numerical model is validated by comparing the temporal conversion profile simulated by the numerical model with ensemble-averaged (~ 5 profiles) conversion profiles obtained from experiments at the laboratory and from literature. The model is validated for different particle sizes, temperature and reactants (air, CO_2 and H_2O). The conversion profile are shown in Figure 2.

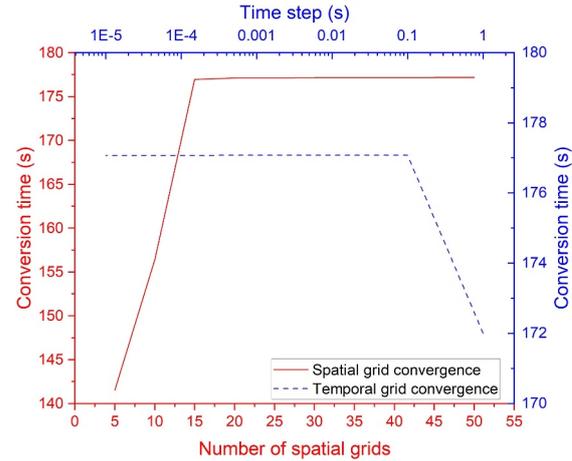


Figure 3: Spatial and temporal grid convergence

Methodology

To assess the influence of diffusivity, simulation results from spatio-temporally evolving diffusivity (using Chapman-Enskog equation and Lennard-Jones potentials) are compared with results from assumed Le consideration. Two cases are considered,

1. A common diffusivity coefficient for all specie derived by assuming unity Lewis number.
2. Specie specific diffusivity coefficient derived by assuming a constant, non-unity Lewis number. The constants are chosen from the works of Smooke and Givangoli; $Le_{O_2} = 1.11$, $Le_{CO_2} = 1.39$, $Le_{CO} = 1.10$, $Le_{H_2} = 0.3$, $Le_{H_2O} = 0.83$, $Le_{N_2} = 1.0$, and $Le_{CH_4} = 0.97$.

The analysis is carried out for an 8 mm diameter char particle subjected to three thermochemi-

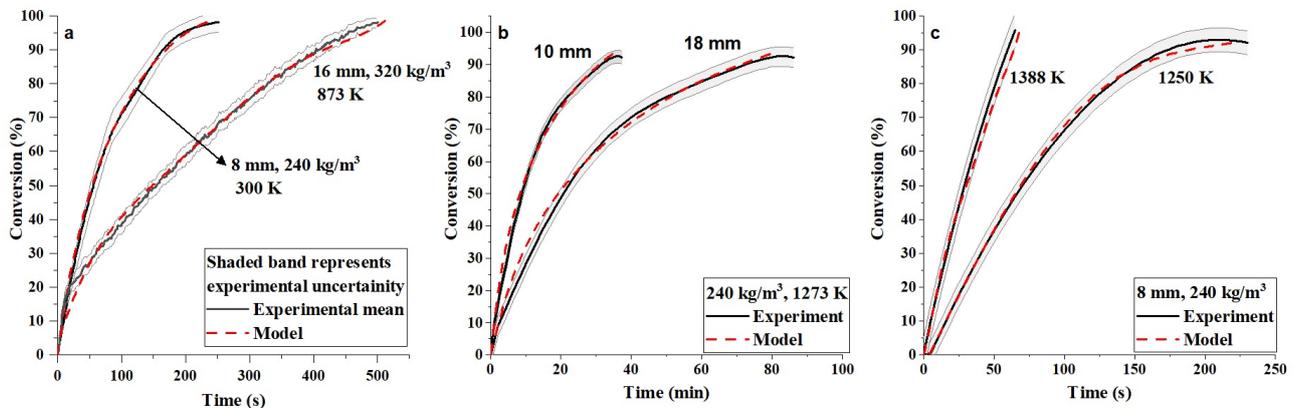


Figure 2: Model validation for char conversion in (a) air (b) CO_2 , (c) H_2O [16].

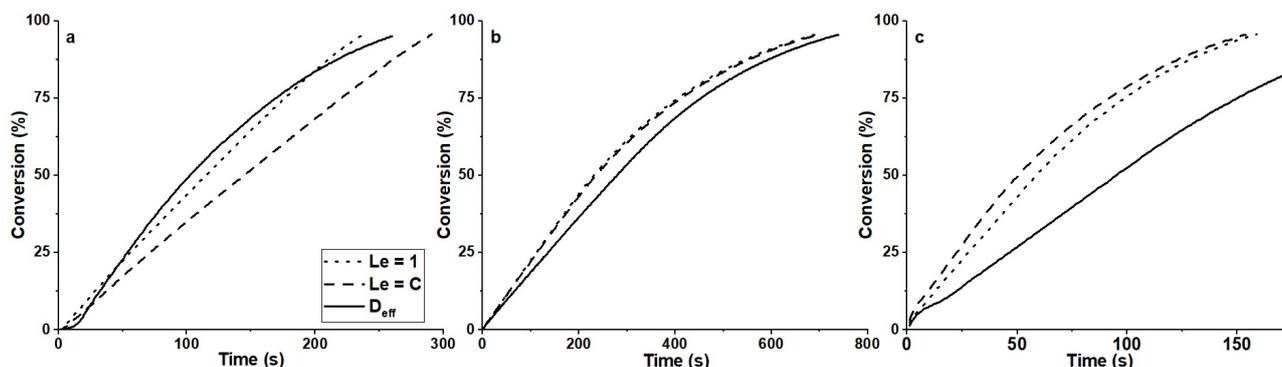


Figure 4: Influence of Le on conversion time and profile (a) char conversion in air (b) char conversion in CO_2 (c) char conversion in H_2O

cal conditions, (i) char conversion in air, initialized at 800 K with ambient of 300 K, (ii) char conversion in CO_2 with both ambient and initialization at 1273 K and (iii) char conversion in steam with ambient and initialization at 1250 K. The influence of Lewis number on the overall conversion behaviour is presented first. Further, the actual variation of Le within the particle as opposed to constant Le is discussed. Towards the end, the variation in intra-particle temperature and reactant concentration due to Le is analyzed.

Results and discussion

Influence of Le on overall conversion behaviour

The conversion profile, conversion with time, is mapped for the two cases discussed above and shown in Figure 4. For char conversion in air (Figure 4a), at 90% conversion, there is a deviation of 5.4% under-prediction when unity Le is assumed and 19.5% over-prediction when constant Le is considered. In both the cases, it can be observed that the nature of conversion profile is significantly different from the actual profile. This is possibly because char conversion in air is a mass diffusion dominated process [16] and any perturbation in the diffusive flux significantly alters the conversion behaviour.

In case of char conversion in CO_2 (Figure 4b), small deviation of 7.3% for constant Le and 7.9% for unity Le is observed at 90% conversion, and the conversion profiles are similar. Since char conversion in CO_2 is a kinetic limited process [11], variation in Le and thereby variation in

diffusive mass flux doesn't significantly influence the conversion behaviour.

Considerable deviations are observed for char conversion in steam (Figure 4c), with 30.8% deviation at 90% conversion for unity Le and 32% deviation for constant Le considered. The products generated as a result of char steam reaction is rich in H_2 (up to 50%) thereby significantly altering the mixture diffusivity leading to the observed deviations.

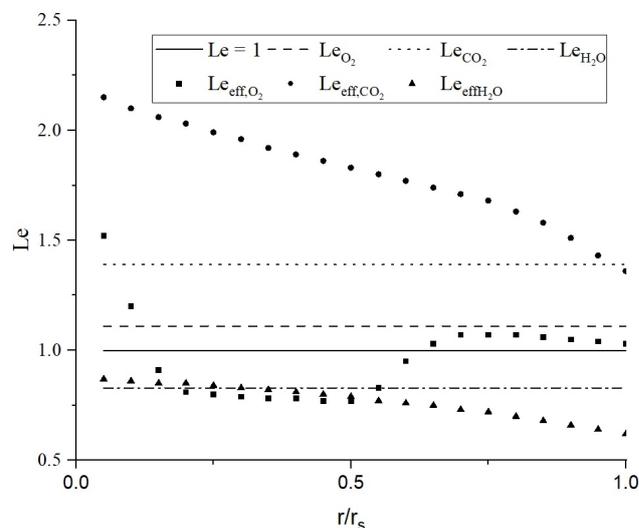


Figure 5: Variation of Le across the particle (normalized radius (r/r_s))

Intra-particle Le assessment

To further understand the heat and mass diffusion processes within the particle, Le as obtained from instantaneous magnitudes of thermal and mass diffusion coefficients across the particle at an instance of 50% particle conversion is ana-

lyzed. The Le estimated from instantaneous values, along with constant Le and unity Le is shown in Figure 5.

It can be observed that in all thermochemical conditions considered (char conversion in O_2 (Air), CO_2 and H_2O), Le is significantly varying across the particle and is far from being constant or unity. Comparing Le at the surface of the particle to its core, in case of CO_2 and H_2O , Le varies by 36% and 28.7% respectively. It can also be seen that Le increases towards the core of the particle. Since char conversion in CO_2 and H_2O are simulated in a high temperature ambient due to their endothermic nature, there is a potential thermal gradient from surface to the core, the thermal gradient influences the thermo-physical properties and thereby Le . It is also to be noted that, in case of CO_2 Le deviates away from unity towards the core, while in case of H_2O Le deviates away from unity towards the surface. This is possibly due to mixture composition, while in case of char- CO_2 reaction, towards the surface the mixture is rich in CO resulting in near unity Le , in case char- H_2O reaction, the mixture towards the surface is rich in H_2 , the higher diffusivity of H_2 lowers the Le away from unity.

In case of char conversion in air, near unity Le is observed towards the surface this is because of the product $CO - CO_2$ mixture having a near unity Le . At the midsection of the particle there is a dip in Le , this is due to the existence of the rapid and highly exothermic reaction zone. The core of the particle initialized at low temperature and unaffected by the reaction front has greater than unity Le .

Variation in intra-particle temperature and reactant distribution due to Le

The stark variation of Le across the particle seen above potentially alters the reactant distribution and thereby the temperature profile. These variations in case of char conversion in air, CO_2 and H_2O are shown in figure 6.

It can be seen in Figure 6a that for char conversion in air, the reactant profile is intermediate of unity Le and constant Le , this is in-line with the Le distribution seen in Figure 5, whose spatial average is 1.03 nearly in mid of unity Le and constant Le (1.11). char-air reaction being mass diffusion dominated, the reaction and thereby the resulting temperature distribution is analogous to the reactant profile.

In case of char conversion in steam, the actual reactant distribution is up to 26% lower than the reactant distribution obtained from unity Le . Since H_2 ($Le \sim 0.3$) constitutes a significant fraction of the mixture in this case, assuming unity Le and deriving diffusivity coefficients from it, over-predicts the estimate, leading to the observed deviation. Further, since the reaction is endothermic, reduced reactant in actual case results in reduced reaction rate and lesser energy absorbed, leading to a higher temperature profile. Similarly, in case of char conversion in CO_2 , the actual reactant distribution is 31.3% lower than the reactant distribution obtained from unity Le consideration. The reduced reactant distribution is attributed to the inability of CO_2 molecule to penetrate the char pores[11]. Like in case of air, lower reactants lead to reduced reaction rate and higher temperature distribution due to endothermicity.

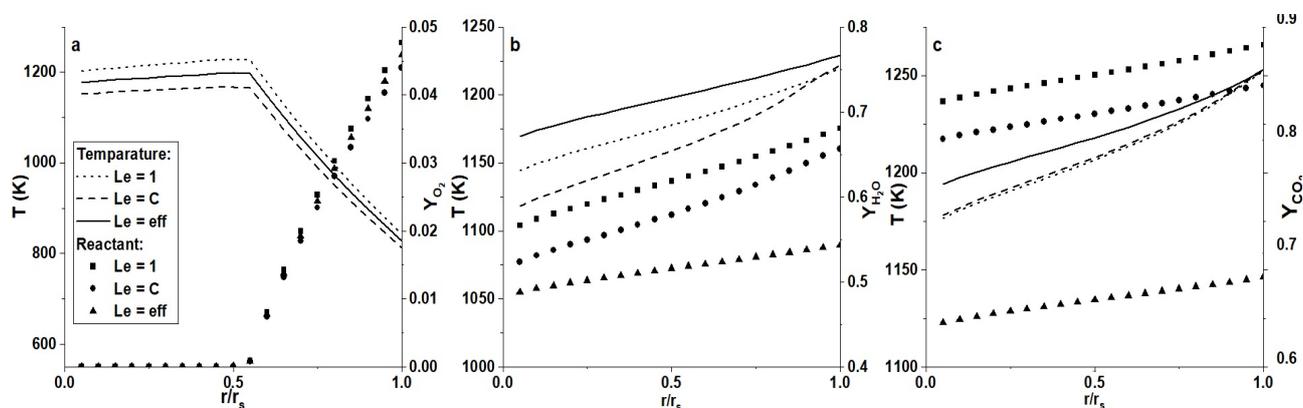


Figure 6: Intra-particle reactant and temperature distribution at 50% particle conversion (a) char conversion in air, (b) char conversion in CO_2 , (c) char conversion in H_2O .

Conclusion

Numerical models for thermochemical conversion of char are often simplified by invoking the Lewis number assumption to simplify the system of equations. The article accesses the potential deviation introduced in simulation results due to the use of diffusivity coefficient derived from an assumed Le as opposed to diffusivity coefficient derived from kinetic theory-based equations. It is found that,

- Lewis number varies significantly across the particle.
- In mass diffusion limited conversion processes, even small perturbation in Le significantly alters the conversion behaviour.
- In kinetically limited conversion process nominal influence of Le is observed on the conversion process.
- Heterogeneous conversion processes tend to be highly sensitive to Le if the evolving gas mixture is rich in H_2 .
- The diffusion coefficient of species within the porous media are significantly small, especially for CO_2 . Under these conditions deriving diffusivity from assumed Le is potentially extraneous.

Assuming constant/unity Le severely deviates the intra-particle reactant concentration, leading to altered reaction rates, temperature distribution and the overall conversion. As such, it is strongly recommended to avoid such assumptions.

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