



# Modeling and simulation of bubbling fluidized bed reactors using a dynamic one-dimensional two-fluid model: The sorption-enhanced steam–methane reforming process



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## ABSTRACT

A dynamic one-dimensional multicomponent model for two-phase flows which includes heat- and mass transfer processes are studied in the Euler framework. The model is intended for reactive gas–solid flows in bubbling fluidized bed reactors. A model is desired that allows for a more complex description of the fluidized bed reactors (e.g. prediction of the bed expansion) relative to the conventional fluidized bed reactor models such as, e.g., Kunii–Levenspiel type of models. The model should not predict details in the flow as the two- and three-dimensional Euler two-fluid models in order to ensure reasonable simulation costs. In particular, the two- and three-dimensional Euler two-fluid models challenges the current available computational capacity for studies of reactive flows.

The novel sorption-enhanced steam methane reforming (SE-SMR) technology is simulated in the bubbling bed regime. Simulation results of the one-dimensional Euler two-fluid model is compared to both a two-dimensional Euler model and a conventional fluidized bed model consisting of mass and heat balances. Furthermore, a sensitivity study to operation conditions and transport coefficients is performed for the one-dimensional Euler two-fluid model.

The present simulation results reveal that the chemical process performance of the reactor is to a large extent determined by the imposed temperature in the reactor. Further, the one-dimensional Euler model provides an improvement of the simpler conventional fluidized bed reactor models by prediction of the bed expansion. Compared with the two-dimensional Euler model, cross-sectional averaging results in a significant reduction in the computational time but on the cost of loss of flow details.

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## 1. Introduction

Hydrogen is currently an important industrial raw material in a number of chemical-, petroleum- and metallurgical processes. Presently, large-scale hydrogen production is mainly dominated by steam reforming of fossil fuels such as natural gas, oil and coal [1]. Steam reforming of natural gas is known as steam methane reforming (SMR) because methane is the major component in natural gas.

A concept called sorption-enhanced reaction process has been introduced in hydrogen production. In this concept, a functionality material is used as sorbent to capture CO<sub>2</sub>. Due to the in situ CO<sub>2</sub> removal, steam reforming of fossil fuels tends towards increased hydrogen production in accordance to the Le Chatelier's principle. The combination of the sorption-enhanced reaction with the SMR process is known as SE-SMR [2–21].

Whereas the SMR process is conventionally operated in fixed packed bed type of reactors, fluidized bed type of reactors, and particularly circulating fluidized bed reactors, are considered suitable for carrying out the SE-SMR technology. In fluidized beds, the solid particles are suspended in an upward flowing stream of gas. At sufficiently high fluid velocities, the frictional force between solid particles and the fluid counterbalances the weight of the solid particles. In this state, the solid particles are referred to as fluidized because they exhibit a fluid-like behavior. Increasing the gas flow rate beyond the point of minimum fluidization, the fluidized bed reactors can be operated in various fluidization regimes. In view of chemical reaction processes, fluidized bed reactors are particularly suitable for highly exothermic and temperature-sensitive reactions since the solid particle motion gives them a unique ability to rapidly transport heat and maintain a uniform temperature. Moreover, the solid particles can easily be replaced which makes the reactors applicable for rapid particle deactivating processes, such as in the SE-SMR technology [22]. A regeneration step where

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**Nomenclature**

*Latin letters*

$A$  problem coefficient matrix of the discretization  
 $A$  prefactor in reaction rate expressions  
 $a$  coefficient of the discretization  
 $a'$  coefficient of the discretization  
 $C_p$  heat capacity, J/(kg K)  
 $B$  coefficient used in PEA; heat balances  
 $b$  coefficient of the discretization; source term  
 $b'$  coefficient of the discretization; source term  
 $d_k$  velocity correction coefficient of phase  $k$   
 $D$  mass dispersion coefficient  
 $D_{ir}$  binary diffusion coefficient,  $m^2/s$   
 $\mathcal{D}$  coefficient used in PEA; momentum balances  
 $D_{g,i}^m$  Wilke diffusion coefficient,  $m^2/s$   
 $D_k$  sub-matrix of matrix  $A$  holding the coupling terms  
 $d$  diameter, m  
 $E$  activation energy  
 $\mathcal{F}$  coefficient used in PEA; generalized  
 $f^f$  fanning friction factor  
 $F$  convective flux,  $kg/(m^2 s)$   
 $g$  gas  
 $g_z$  gravity,  $m/s^2$   
 $G$  modulus of elasticity,  $kg/(s^2 m)$   
 $\Delta H$  heat of reaction, J/kmol  
 $H$  height of reactor bed, m  
 $H_{mf}$  height of solid in the reactor bed at minimum fluidization, m  
 $h_{gs}$  interfacial heat transfer coefficient,  $kg/(s^3 K)$   
 $I$  generic flux  
 $k$  rate coefficient in reaction rate equations  
 $k$  generalized phase index,  $k = g, s$   
 $k$  heat conductivity,  $J/(m s K)$   
 $K$  generalized proportional coefficient in inter-phase flux term  
 $K$  adsorption constants in reaction rate equations  
 $l$  generalized phase index,  $l \neq k$   
 $M$  molecular mass,  $kg/kmol$   
 $\max(a, b)$  maximum of  $a, b$   
 $\mathcal{M}_k$  inter-phase momentum transfer,  $kg/(m^2 s^2)$   
 $p_g$  gas phase pressure, Pa  
 $p_g^{\text{correction}}$  gas phase pressure correction, Pa  
 $p_g^*$  guessed gas phase pressure, Pa  
 $Q^i$  interfacial heat transfer,  $J/(m^3 s)$   
 $R$  gas constant,  $J/(kmol K)$   
 $R_{rx_i}$  reaction rate of reaction  $rx_i$ ,  $kmol/(m^3 s)$   
 $R_{k,i}$  formation rate of species  $i$  in phase  $k$ ,  $kmol/(m^3 s)$   
 $Re$  Reynolds number, dimensionless  
 $t$  time, s  
 $\Delta t$  time step, s  
 $T$  temperature, K  
 $s$  solid  
 $S$  generalized source term  
 $S$  heat source term in the two-phase model  
 $S^C$  source term independent of the dependent variable  
 $S^\varphi$  source term coefficient dependent on the dependent variable  
 $S$  specific surface area  
 $v_k$  velocity of phase  $k$ , m/s  
 $v_k^{\text{correction}}$  velocity correction of phase  $k$ , m/s  
 $v_k^{\text{corrected}}$  corrected phase  $k$  velocity due to pressure, m/s  
 $X$  fractional conversion of sorbent

$z$  axial reactor dimension, m  
 $\Delta z$  axial resolution, m

*Greek letters*

$\Gamma_k$  inter-phase mass transfer flux,  $kg/(m^3 s)$   
 $\epsilon_k$  cross-sectional area fraction of phase  $k$   
 $\rho$  density,  $kg/m^3$   
 $\rho^*, \rho^{**}, \rho^{***}$  density estimates by fractional step  
 $\tau$  shear stress,  $kg/(s^2 m)$   
 $\omega$  species mass fraction  
 $\varphi$  generalized property  
 $\mathcal{A}$  generalized diffusion coefficient  
 $\epsilon_{iter}$  relative iteration error  
 $\epsilon_{res}$  residual error  
 $\gamma$  defined by Eq. (44),  $kg/(K s^3 m)$   
 $\mu$  viscosity,  $kg/(m s)$   
 $\beta$  inter-phase drag coefficient  
 $\phi$  pellet sphericity

*Subscript*

$CO_2$  carbon dioxide  
 $e$  east interfacial node  
 $E$  east node  
 $g$  gas  
 $i$  species type  
 $j$  grid index, velocity node  
 $J$  grid index, scalar node  
 $k$  phase,  $k = g, s$   
 $l$  phase,  $l \neq k$   
 $mf$  minimum fluidization  
 $nb$  neighbor node  
 $rx_i$  reaction index  
 $s$  solid  
 $t$  tube, reactor bed  
 $P$  central node  
 $p$  solid particle  
 $wall$  reactor bed wall  
 $w$  west interfacial node  
 $W$  west node

*Superscript*

Cap  $CO_2$  capture reaction  
 $eff$  effective  
 $eq$  equilibrium  
 $i$  interface  
 $in$  reactor entrance  
 $m$  molecular  
 $n$  time level  
 $n$  power number in reaction rate equation for  $CO_2$ -capture at the reactor outlet  
 $out$  at the reactor outlet  
 $SMR$  reaction of the steam methane reforming  
 $stat$  static  
 $t$  turbulent  
 $v$  iteration

*Abbreviation*

PEA partial elimination algorithm  
 $SMR$  steam methane reforming  
 $SE-SMR$  sorption-enhanced steam methane reforming

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