ESI: Comprehensive Overview of the effective thermal conductivity for hydride material: experimental and modeling approaches

Gabriele Scarpati [1], Julián A. Puszkiel [2,3,*], Jan Warfsmann[2,3], Fahim Karimi[2], Elio Jannelli[1], Claudio Pistidda[2], Thomas Klassen[2,3], Julian Jepsen[2]

[1] University of Naples "Parthenope", Naples, Italy; gabriele.scarpati001@studenti.uniparthenope.it
[2] Helmholtz-Zentrum Hereon, Max-Planck-Straße 1, 21502 Geesthacht, Germany
[3] Helmut Schmidt University, University of the Federal Armed Forces Hamburg, Holstenhofweg 85, 22043, Hamburg, Germany

* Correspondence: julian.puszkiel@hereon.de; Tel.: +49(0)415287-2171 / +49(0)406541 3297

<table>
<tr><th>Name</th><th>Year</th><th colspan="2">Main equation and parameters</th><th colspan="2">Main features</th></tr>
<tr><td rowspan="3">3.1.1 Maxwell model [42]: M</td><td rowspan="3">1873</td><td colspan="2">$$k_{eff} = k_g \frac{1+2\frac{\frac{k_s}{k_g}-1}{\frac{k_s}{k_g}+2}(1-\varepsilon)}{1-\frac{\frac{k_s}{k_g}-1}{\frac{k_s}{k_g}+2}(1-\varepsilon)}$$</td><td colspan="2">• Made for solid particles dispersed in a fluid phase (not for MHs)
• There is no finite contact area between adjacent particles
• Applicable for low concentrations of the particulate</td></tr>
<tr><th>Measurable or literature</th><th>Hard to measure or to fit</th><th>Pros</th><th>Cons</th></tr>
<tr><td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
ε (Porosity, if considered constant)</td><td>• ε (Porosity, if not constant)</td><td>• Simple
• A reduced number of parameters
• No hard-to-get parameters</td><td>• Not specific for MH</td></tr>
<tr><td rowspan="3">3.1.2 Yagi and Kunii model [92]: YK</td><td rowspan="3">1957</td><td colspan="2">$$k_{eff} = \frac{l_p(1-\varepsilon)}{\frac{l_s}{k_s}+\frac{l_v}{k_g+l_v h_{rs}}} + \varepsilon l_p h_{rv}$$</td><td colspan="2">• Made for solid particles dispersed in a fluid phase (not for MHs)
• There is no finite contact area between adjacent particles
• Two contributions: one is independent of fluid flow, and the other depends on the lateral mixing of the fluid in the packed beds</td></tr>
<tr><th>Measurable or literature</th><th>Hard to measure or to fit</th><th>Pros</th><th>Cons</th></tr>
<tr><td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
• ε (Porosity, if considered constant)
• l_p (effective length between the centers of two adjacent particles)
• l_s (effective length of the solid particles related to the heat conduction)</td><td>• e (emissivity factor of the solid surface)
• l_v (effective thickness of the fluid film adjacent to the contact surface of two solid particles)
• ε (Porosity, if not constant)</td><td>• Simple
• Limited number of parameters</td><td>• Not specific for MH
• Some parameters are hard to get or remain as fitting parameters</td></tr>
<tr><td rowspan="3">3.1.3 Zehner-Schlünder model [44]: ZS</td><td rowspan="3">1970</td><td colspan="2">$$k_{eff} = k_g \cdot \left(1-\sqrt{1-\varepsilon}+\frac{2\sqrt{1-\varepsilon}}{1-\frac{k_g}{k_s}B}\left(\frac{\left(1-\frac{k_g}{k_s}\right)B}{\left(1-\frac{k_g}{k_s}B\right)^2}\ln\frac{k_s}{k_g B}-\frac{B+1}{2}-\frac{B-1}{1-\frac{k_g}{k_s}B}\right)\right)$$</td><td colspan="2">• Made for solid particles dispersed in a fluid phase (not for MHs)
• There is no finite contact area between adjacent particles
• Two parallel paths for heat conduction, one in the fluid area and one in the biphasic region</td></tr>
<tr><th>Measurable or literature</th><th>Hard to measure or to fit</th><th>Pros</th><th>Cons</th></tr>
<tr><td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
• ε (Porosity, if considered constant)</td><td>• C (Form factor)
• m (Exponential fitting parameter)
• B (Shape factor/alternative to C, m, and ε)
• ε (Porosity, if not constant)</td><td>• A small number of parameters</td><td>• Not specific for MH</td></tr>
<tr><td rowspan="3">3.1.4 Zehner-Bauer-Schlünder model [95-97]: ZBS</td><td rowspan="3">1978</td><td colspan="2">$$k_{eff} = \left(1-\sqrt{1-\varepsilon}\right)k_h + \sqrt{1-\varepsilon}\left((1-\varphi)k_{bp}+\varphi k_s\right)$$</td><td colspan="2">• Made for solid particles dispersed in a fluid phase (not for MHs)
• Finite contact area between adjacent particles
• Three parallel paths for heat conduction: one in the fluid area, one in the biphasic region, and one through solid particles</td></tr>
<tr><th>Measurable or literature</th><th>Hard to measure or to fit</th><th>Pros</th><th>Cons</th></tr>
<tr><td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
• ε (Porosity, if considered constant)
• γ (Specific heat ratio)
• μ_g (Dynamic viscosity of hydrogen)
• c_v (Heat capacity at constant volume)
• l (Mean free path)
• d (Particle diameter)</td><td>• C (Form factor)
• m (Exponential fitting parameter)
• B (Shape factor/alternative to C, m, and ε)
• e (emissivity factor of the solid surface)
• d_c (Contact area diameter)
• a (Accommodation coefficient)
• ε (Porosity, if not constant)</td><td>• Relatively simple
• Contact area</td><td>• Not specific for MH</td></tr>
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<tr>
<td rowspan="3">3.1.5 Hayashi model [43]: H</td>
<td rowspan="3">1987</td>
<td colspan="2">$$k_{eff} = \frac{1}{2}(3\varepsilon - 1)\left(k_{g1} + \beta' h_{rv} d \cos\theta\right) + \frac{3\beta'(1-\varepsilon)(1-\delta)\cos\theta}{2\left(\frac{1}{\frac{k_{g2}}{\phi^*}+h_{rs}d}+\frac{\cos\theta-\phi^*}{k_s}\right)} + \frac{3}{2}(1-\varepsilon)\delta k_s$$</td>
<td colspan="2">• Made for solid particles dispersed in a fluid phase (not for MHs)
• Finite contact area between adjacent particles
• Three parallel paths for heat conduction: one in the fluid area, one in the biphasic region, and one through solid particles</td>
</tr>
<tr>
<td>Measurable or literature</td>
<td>Hard to measure or to fit</td>
<td>Pros</td>
<td>Cons</td>
</tr>
<tr>
<td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
• ε (Porosity, if considered constant)
• k_{e0} (Effective thermal conductivity at zero pressure)
• γ (Specific heat ratio)
• l (Mean free path)
• d (Particle diameter)</td>
<td>• e (emissivity factor of the solid surface)
• n (number of contact points for a hemispherical particle surface)
• a (Accommodation coefficient)
• ε (Porosity, if not constant)</td>
<td>• Contact area
• Good adaptability to different systems</td>
<td>• Not specific for MH
• Some parameters are hard to get or remain as fitting parameters</td>
</tr>
<tr>
<td rowspan="3">3.1.5 Simplified Hayashi model [43]: SH</td>
<td rowspan="3">1987</td>
<td colspan="2">$$k_{eff} = \frac{1}{2}(3\varepsilon - 1)k_{g1} + \frac{3\beta'(1-\varepsilon)(1-\delta)\cos\theta}{2\left(\frac{\phi^*}{k_{g2}}+\frac{\cos\theta-\phi^*}{k_s}\right)} + \frac{3}{2}(1-\varepsilon)\delta k_s$$</td>
<td colspan="2">• Made for solid particles dispersed in a fluid phase (not for MHs)
• Finite contact area between adjacent particles
• Three parallel paths for heat conduction: one in the fluid area, one in the biphasic region, and one through solid particles</td>
</tr>
<tr>
<td>Measurable or literature</td>
<td>Hard to measure or to fit</td>
<td>Pros</td>
<td>Cons</td>
</tr>
<tr>
<td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
• ε (Porosity, if considered constant)
• k_{e0} (Effective thermal conductivity at zero pressure)
• γ (Specific heat ratio)
• l (Mean free path)
• d (Particle diameter)</td>
<td>• n (number of contact points for a hemispherical particle surface)
• a (Accommodation coefficient)
• ε (Porosity, if not constant)</td>
<td>• Contact area
• Good adaptability to different systems</td>
<td>• Not specific for MH
• Some parameters are hard to get or remain as fitting parameters</td>
</tr>
<tr>
<td rowspan="3">3.1.6 Sun and Deng model [46,47]: SD</td>
<td rowspan="3">1990</td>
<td colspan="2">$$k_{eff} = \left(1-\frac{4}{\pi}(1-\varepsilon)\right)\left(k_g^* + r\cdot h_{rv}\right) + \left(\frac{\frac{4}{\pi}(1-\varepsilon)(1-\tan\theta_0)}{\frac{\frac{\pi}{4}-\tan\theta_0}{(1-\tan\theta_0)k_s^*}+\frac{1-\frac{\pi}{4}}{(1-\tan\theta_0)k_g^*+\left(1-\frac{\pi}{4}\right)r\cdot h_{rs}}}\right) + \frac{4}{\pi}(1-\varepsilon)\tan\theta_0\, k_s^*$$</td>
<td colspan="2">• Made for MHs
• Finite contact area between adjacent particles
• Three parallel paths for heat conduction: one in the fluid area, one in the biphasic region, and one through solid particles
• The equation for the hydrogen thermal conductivity (dependent on pressure)
• The equation for the solid phase thermal conductivity (dependent on hydrogen concentration)</td>
</tr>
<tr>
<td>Measurable or literature</td>
<td>Hard to measure or to fit</td>
<td>Pros</td>
<td>Cons</td>
</tr>
<tr>
<td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
• ε (Porosity, if considered constant)
• k_{e0} (Effective thermal conductivity at zero pressure)
• ρ_g (Gas density)
• l (Mean free path)
• d (Particle diameter)</td>
<td>• e (emissivity factor of the solid surface)
• b (Accommodation coefficient)
• ε (Porosity, if not constant)</td>
<td>• Relatively simple
• Contact area
• Made for MH</td>
<td>• Some parameters are hard to get or remain as fitting parameters</td>
</tr>
<tr>
<td>3.1.6 Simplified Sun and Deng model [46,47]: SSD</td>
<td></td>
<td colspan="2">$$k_{eff} = \left(1-\frac{4}{\pi}(1-\varepsilon)\right)k_g^* + \left(\frac{\frac{4}{\pi}(1-\varepsilon)(1-\tan\theta_0)}{\frac{\frac{\pi}{4}-\tan\theta_0}{(1-\tan\theta_0)k_s^*}+\frac{1-\frac{\pi}{4}}{(1-\tan\theta_0)k_g^*}}\right) + \frac{4}{\pi}(1-\varepsilon)\tan\theta_0\, k_s^*$$</td>
<td colspan="2">• Made for MHs
• Finite contact area between adjacent particles
• Three parallel paths for heat conduction: one in the fluid area, one in the biphasic region, and one through solid particles
• The equation for the hydrogen thermal conductivity (dependent on pressure)</td>
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<tr><td rowspan="3"></td><td rowspan="3">1990</td><td colspan="2"></td><td colspan="2">• The equation for the solid phase thermal conductivity (dependent on hydrogen concentration)</td></tr>
<tr><td>Measurable or literature</td><td>Hard to measure or to fit</td><td>Pros</td><td>Cons</td></tr>
<tr><td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
• ε (Porosity, if considered constant)
• k_{e0} (Effective thermal conductivity at zero pressure)
• ρ_g (Gas density)
• l (Mean free path)
• d (Particle diameter)</td><td>• b (Accommodation coefficient)
• ε (Porosity, if not constant)</td><td>• Contact area
• Made for MH
• It is simpler than the base model</td><td>• Some parameters are hard to get or remain as fitting parameters</td></tr>
<tr><td rowspan="3">3.1.7 Extended Zehner-Bauer-Schlünder model [95]: EZBS</td><td rowspan="3">1994</td><td colspan="2">$$k_{eff} = \left(1-\sqrt{1-\varepsilon}\right)k_h + \sqrt{1-\varepsilon}\left((1-\varphi)k_{bp} + \varphi k_s\right)$$</td><td colspan="2">• Made for MHs
• Finite contact area between adjacent particles
• Three parallel paths for heat conduction: one in the fluid area, one in the biphasic region, and one through solid particles
• The equation for the solid phase thermal conductivity (dependent on hydrogen concentration)
• The equation for the porosity (dependent on hydrogen concentration)</td></tr>
<tr><td>Measurable or literature</td><td>Hard to measure or to fit</td><td>Pros</td><td>Cons</td></tr>
<tr><td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
• ε (Porosity, if considered constant)
• γ (Specific heat ratio)
• μ_g (Dynamic viscosity of hydrogen)
• c_v (Heat capacity at constant volume)
• l (Mean free path)
• d (Particle diameter)
• ρ_s (density of the metal)
• x_{max} (Maximum hydrogen to metal concentration)
• E (Young's modulus)
• ν (Poisson's ratio)
• r_0 (initial particle radius)</td><td>• e (emissivity factor of the solid surface)
• a (Accommodation coefficient)
• B (Shape factor)
• $r_{c,0}$ (Initial contact area radius)
• ε (Porosity, if not constant)</td><td>• Adapted for MH beds
• Many equations are given for several parameters</td><td>• Quite complex
• Some parameters need to be evaluated experimentally</td></tr>
<tr><td rowspan="3">3.1.8 Modified Zehner-Schlünder: area-contact model [45]: AC</td><td rowspan="3">1994</td><td colspan="2">$$k_{eff} = \left(1-\sqrt{1-\varepsilon}\right)k_g + k_s\sqrt{1-\varepsilon}\left(1-\frac{1}{(1+\alpha B)^2}\right) + \frac{2k_g\sqrt{1-\varepsilon}}{1-\frac{k_g}{k_s}B+\left(1-\frac{k_g}{k_s}\right)\alpha B} \cdot$$ $$\cdot\left(\frac{\left(1-\frac{k_g}{k_s}\right)(1+\alpha)B}{\left(1-\frac{k_g}{k_s}B+\left(1-\frac{k_g}{k_s}\right)\alpha B\right)^2}\cdot\ln\frac{1+\alpha B}{(1+\alpha)B\frac{k_g}{k_s}} - \frac{B+1+2\alpha B}{2(1+\alpha B)^2} - \frac{B-1}{\left(1-\frac{k_g}{k_s}B+\left(1-\frac{k_g}{k_s}\right)\alpha B\right)(1+\alpha B)}\right)$$</td><td colspan="2">• Made for solid particles dispersed in a fluid phase (not for MHs)
• Finite contact area between adjacent particles
• Three parallel paths for heat conduction: one in the fluid area, one in the biphasic region, and one through solid particles</td></tr>
<tr><td>Measurable or literature</td><td>Hard to measure or to fit</td><td>Pros</td><td>Cons</td></tr>
<tr><td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
• ε (Porosity, if considered constant)</td><td>• C (Form factor)
• m (Exponential fitting parameter)
• B (Shape factor/alternative to C, m, and ε)
• α (Deformed factor)
• ε (Porosity, if not constant)</td><td>• A reduced number of parameters
• Contact area</td><td>• Not specific for MH</td></tr>
</table>

<table>
<tr><td rowspan="3">3.1.9 Modified Zehner-Schlünder: phase-symmetry model [45]: PS</td><td rowspan="3">1994</td><td colspan="2">$$k_{eff} = k_g\left(1-\sqrt{1-\varepsilon}\right) + k_s\left(1-\sqrt{\varepsilon}\right) + k_g\left(\sqrt{1-\varepsilon}+\sqrt{\varepsilon}-1\right)\left(\frac{B\left(1-\frac{k_g}{k_s}\right)}{\left(1-\frac{k_g}{k_s}B\right)^2} ln\frac{k_s}{k_g B} - \frac{B-1}{1-\frac{k_g}{k_s}B}\right)$$</td><td colspan="2">• Made for sponge-like porous materials, with each phase continuously connected and in phase symmetry (not for MHs)
• Three parallel paths for heat conduction: one in the fluid area, one in the biphasic region, and one through solid particles</td></tr>
<tr><td>Measurable or literature</td><td>Hard to measure or to fit</td><td>Pros</td><td>Cons</td></tr>
<tr><td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
• ε (Porosity, if considered constant)</td><td>• B (Shape factor, alternative to ε)
• ε (Porosity, if not constant)</td><td>• A small number of parameters</td><td>• Not specific for MH</td></tr>
<tr><td rowspan="3">3.1.10 Raghavan-Martin model [49]: RM</td><td rowspan="3">1995</td><td colspan="2">$$k_{eff} = k_g\left(1+\frac{1-\varepsilon}{\frac{\frac{k_s}{k_g}}{\frac{k_s}{k_g}-1} - h_{Maxwell}\cdot Z}\right)$$</td><td colspan="2">• Made for solid particles dispersed in a fluid phase (not for MHs)
• There is no finite contact area between adjacent particles</td></tr>
<tr><td>Measurable or literature</td><td>Hard to measure or to fit</td><td>Pros</td><td>Cons</td></tr>
<tr><td>• k_s (Solid phase (bulk) thermal conductivity)
• k_g (Gas (hydrogen) thermal conductivity)
• ε (Porosity, if considered constant)</td><td>• A_0 (Fitting parameter)
• A_1 (Fitting parameter)
• ε (Porosity, if not constant)</td><td>• Simple
• A reduced number of parameters</td><td>• Not specific for MH</td></tr>
<tr><td rowspan="3">3.1.11 Improved area-contact model [50]: IAC</td><td rowspan="3">2014</td><td colspan="2">$$k_{eff} = \left(1-\sqrt{1-\varepsilon}\right)k_g + \sqrt{1-\varepsilon}\left(1-\frac{1}{(1+\alpha_a B_a)^2}\right)k_s + \frac{2k_g\sqrt{1-\varepsilon}}{1-\frac{k_g}{k_s}B_a+\left(1-\frac{k_g}{k_s}\right)\alpha_a B_a}\cdot$$ $$\cdot\left(\frac{\left(1-\frac{k_g}{k_s}\right)(1+\alpha_a)B_a}{\left(1-\frac{k_g}{k_s}B_a+\left(1-\frac{k_g}{k_s}\right)\alpha_a B_a\right)^2}\cdot ln\frac{1+\alpha_a B_a}{(1+\alpha_a)B_a\frac{k_g}{k_s}} - \frac{B_a+1+2\alpha_a B_a}{2(1+\alpha_a B_a)^2} - \frac{B-1}{\left(1-\frac{k_g}{k_s}B_a+\left(1-\frac{k_g}{k_s}\right)\alpha_a B_a\right)(1+\alpha_a B_a)}\right)$$</td><td colspan="2">• Made for MHs
• Finite contact area between adjacent particles
• Three parallel paths for heat conduction: one in the fluid area, one in the biphasic region, and one through solid particles
• Equations for particle deformation during cycles are included
• The equation for the hydrogen thermal conductivity (dependent on the hydrogen viscosity, specific heat capacity at constant pressure, and mean free path, so on temperature and pressure)
• The equation for the porosity (dependent on hydrogen concentration)</td></tr>
<tr><td>Measurable or literature</td><td>Hard to measure or to fit</td><td>Pros</td><td>Cons</td></tr>
<tr><td>• k_s (Solid phase (bulk) thermal conductivity)
• ε_0 (Initial porosity)
• d_0 (Initial particle diameter)
• l (Mean free path)
• γ (Specific heat ratio)
• μ (Dynamic viscosity)
• c_p (Heat capacity at constant pressure)
• V_0 (Minimum MH bed volume)
• V_1 (Maximum MH bed volume)
• V_2 (MH bed volume at the end of the cycle)
• ϕ_p (Particle expansion ratio)</td><td>• a (Accommodation coefficient)
• α_0 (Initial deformed factor)
• B_0 (Initial shape factor)
• α_a or B_a (Shape factor after the expansion)
• P_{eq} (Equilibrium pressure)
• R_P (Reacted fraction at the beginning of the plateau)
• ε (Porosity, if not constant)</td><td>• Detailed
• Made for MHs</td><td>• Complex
• A high number of parameters
• Some parameters are hard to get or remain as fitting parameters</td></tr>
<tr><td>3.1.12 Abdin-Webb-Gray model [102]: AWG</td><td>2018</td><td colspan="2">$$k_{eff} = \frac{N(1-\varepsilon)}{\pi d\cdot R_c}$$</td><td colspan="2">• Made for MH bes
• The contact between two particles can be divided into two different scale regions: the macro-gap and the micro-gap
• Four thermal resistances are involved: that of the gas (RG), related to the perfect contact between particles (RL), that related to micro-contacts (Rs), and that of the interstitial gas contained in the micro-gaps (Rg)
• Many of the parameters are solid mechanical properties</td></tr>
</table>

				• The equation for the hydrogen thermal conductivity (dependent on the hydrogen mean free path, so on temperature and pressure) • The equation for the porosity (dependent on hydrogen concentration)	
		Measurable or literature	**Hard to measure or to fit**	**Pros**	**Cons**
		• k_s (Solid phase (bulk) thermal conductivity) • $k_{g,ref}$ (Gas (hydrogen) thermal conductivity at reference pressure) • ε_0 (Initial porosity) • d_0 (Initial particle diameter) • γ (Specific heat ratio) • V_0 (Minimum MH bed volume) • V_1 (Maximum MH bed volume) • V_2 (MH bed volume at the end of the cycle) • Pr (Prandtl number) • ϕ_p (Particle expansion ratio)	• d_v (Mean indentation diagonal depth) • C_1 (Vickers microhardness coefficient 1) • C_2 (Vickers microhardness coefficient 2) • E' (Effective Young's modulus) • σ_R (Surface roughness) • α_{T1} (Thermal accommodation coefficient 1) • α_{T2} (Thermal accommodation coefficient 2) • P_{eq} (Equilibrium pressure) • R_P (Reacted fraction at the beginning of the plateau) • ε (Porosity, if not constant)	• Detailed • Made for MHs • Interesting mechanical approach	• Complex • A high number of parameters • Some parameters are hard to get or remain as fitting parameters
***3.1.13 Heat transfer concentrating model* [91]: HTC**	**2023**	$k_{eff} = \frac{k_s k_g\left(\frac{\varepsilon}{G}+1-\varepsilon\right)}{\frac{\varepsilon}{G}\cdot k_s+k_g(1-\varepsilon)}$		• Made for solid particles dispersed in a fluid phase (not for MHs) • Only one not-negligible path for heat conduction, that in the biphasic region	
***3.1.13 Heat transfer concentrating model* [91]: HTC**	**2023**	**Measurable or literature**	**Hard to measure or to fit**	**Pros**	**Cons**
***3.1.13 Heat transfer concentrating model* [91]: HTC**	**2023**	• k_s (Solid phase (bulk) thermal conductivity) • k_g (Gas (hydrogen) thermal conductivity) • ε (Porosity, if considered constant) • d (Particle diameter)	• ε (Porosity, if not constant)	• Simple • A reduced number of parameters	• Not made for MHs

Table S1. Summary of the models with the central equation, brief description, parameters and advantages and disadvantages.

Name	Solid material	Fluid	Parameters	Values			T-P exp. ranges	
***3.1.1 Maxwell model* [42]: M**				LaNi$_5$-air	Fe-air		T (K)	P (bar)
	• LaNi$_5$ • Fe	• Air	• k_s • k_g • ε	• 12.5 W/(m·K) • 0.0258 W/(m·K) • 0.468-0.669	• 79 W/(m·K) • 0.0258 W/(m·K) • 0.546-0.681		293.15	1.01325
	k_{eff} ranges **(Exp. to model deviation > 50 %)**		• **Exp.** • **Model**	• **0.1187-0.2288 W/(m·K)** • **0.0637-0.1127 W/(m·K)**	• **0.1302-0.2317 W/(m·K)** • **0.0621-0.0900 W/(m·K)**			
***3.1.2 Yagi and Kunii model* [92]: YK**				Iron sphere-air	Porcelain granule-air	Cement clinker-air	T (K)	P (bar)
	• Iron sphere • Porcelain cylinder • Porcelain granule • Cement clinker • Insulating fire brick • Raschig ring	• Air	• k_s • k_g • ε • l_p • l_s • l_v • e	• 52.3 W/(m·K) • 0.0211-0.0696 W/(m·K) • 0.4 • 11 mm • 11 mm • 0.374 mm • Not reported	• 1.63 W/(m·K) • 0.0211-0.0696 W/(m·K) • 0.43 • 6 mm • 6 mm • 0.24 mm • Not reported	• 1.98 W/(m·K) • 0.0211-0.0696 W/(m·K) • 0.5 • 2.6 mm • 2.6 mm • 0.12 mm • Not reported	423.15-1123.15	1.01325
	k_{eff} ranges **(Exp. to model deviation < 15 %)**		• **Exp.** • **Model**	• **0.707-3.85 W/(m·K)** • **0.806-3.40 W/(m·K)**	• **0.519-1.39 W/(m·K)** • **0.511-1.42 W/(m·K)**	• **0.384-0.889 W/(m·K)** • **0.362-0.807 W/(m·K)**		
***3.1.3 Zehner-Schlünder model* [44]: ZS**				Bronze-water	Bronze-air	Aluminium-air	T (K)	P (bar)
	• Glass • Stainless steel • Urea-formaldehyde • Bronze • Aluminium	• Water • Glycerol • Air	• k_s • k_g • C • m • ε	• 117 W/(m·K) • 0.623 W/(m·K) • 1.25 • 10/9 • 0.4	• 117 W/(m·K) • 0.0268 W/(m·K) • 1.25 • 10/9 • 0.39	• 218 W/(m·K) • 0.0268 W/(m·K) • 1.25 • 10/9 • 0.41	308.15	Not indicated
	k_{eff} ranges **(Exp. to model deviation < 80 %)**		• **Exp.** • **Model**	• **4.61 W/(m·K)** • **7.32 W/(m·K)**	• **1.23 W/(m·K)** • **0.628 W/(m·K)**	• **3.89 W/(m·K)** • **0.706 W/(m·K)**		
***3.1.4 Zehner-Bauer-Schlünder model* [95-97]: ZBS**				LaNi$_{4.7}$Al$_{0.3}$-H$_2$	HWT 5800-H$_2$		T (K)	P (bar)
	• LaNi$_{4.7}$Al$_{0.3}$ (not activated) • HWT 5800 (not activated)	• Ar • He • N$_2$ • H$_2$	• k_s • k_g • C • m • ε • γ • μ_g • c_v • l • e • d • d_c • a	• 12.5 W/(m·K) • 0.18 W/(m·K) • 1.4 • 10/9 • 0.531 • Not reported • Not reported • Not reported • Not reported • Not reported • 36 μm • 0.1548 μm • 0.5	• 12 W/(m·K) • 0.18 W/(m·K) • 1.4 • 10/9 • 0.445 • Not reported • Not reported • Not reported • Not reported • Not reported • 50 μm • 0.075 μm • 0.5		293.15	10^{-5}-100
	k_{eff} ranges **(Exp. to model deviation < 30 %)**		• **Exp.** • **Model**	• **0.00426-1.34 W/(m·K)** • **0.00339-1.10 W/(m·K)**	• **0.00454-1.89 W/(m·K)** • **0.00593-1.54 W/(m·K)**			
***3.1.5 Hayashi model* [43]: H** and				Activated alumina-H$_2$	Glass beads-H$_2$	Lead balls-H$_2$	T (K)	P (bar)
	• Glass beads • Lead balls • Activated alumina • Cylindrical PVC resin	• He • H$_2$ • N$_2$ • Ar • C$_3$H$_6$	• k_s • k_g • k_{e0} • ε • γ	• 0.455 W/(m·K) • Not reported • 0.00814 W/(m·K) • 0.404 • Not reported	• 1.035 W/(m·K) • Not reported • 0.0174 W/(m·K) • 0.4 • Not reported	• 34.9 W/(m·K) • Not reported • 0.0464 W/(m·K) • 0.42 • Not reported	288.15-293.15	0.0133-1.013

3.1.5 Simplified Hayashi model **[43]: SH**		• He-N_2 mixture	• d • n • e • *l* • a	• 0.23 mm • Not reported • Not reported • Not reported • ≈ 0.5	• 0.462 mm • Not reported • Not reported • Not reported • ≈ 0.5	• 1.1 mm • Not reported • Not reported • Not reported ≈ 0.5		
	k_{eff} ranges **(Exp. to model deviation < 20 %, expect at low ranges for activated alumina-H_2)**		• **Exp.** • **Model**	• **0.00225-0.331 W/(m·K)** • **0.00500-0.322 W/(m·K)**	• **0.0247-0.558 W/(m·K)** • **0.0194-0.557 W/(m·K)**	• **0.0549-1.81 W/(m·K)** • **0.0555-1.75 W/(m·K)**		
				$MlNi_{4.5}Mn_{0.5}$-H_2			T (K)	P (bar)
3.1.6 Sun and Deng model **[46,47]: SD** and ***3.1.6 Simplified Sun and Deng model*** **[46,47]: SSD**	• $MlNi_{4.5}Mn_{0.5}$	• H_2	• k_s • k_g • k_{e0} • ε • e • d • ρ_g • l • a • b	• Not reported • Not reported • Not reported • Not reported • 0.9 • 25 µm • Not reported • Not reported • Not reported • Not reported			313.15-333.15	1-40
	k_{eff} ranges **(Exp. to model deviation < 5 %)**		• **Exp.** • **Model**	• **0.714-1.29 W/(m·K)** • **0.754-1.27 W/(m·K)**				
				$LaNi_{4.7}Al_{0.3}$-H_2	HWT 5800-H_2		T (K)	P (bar)
3.1.7 Extended Zehner-Bauer-Schlünder model **[95]: EZBS**	• $LaNi_{4.7}Al_{0.3}$ • HWT 5800	• H_2	• $k_{s,0}$ • k_g • ε_0 • C • m • γ • μ_g • c_v • *l* • e • $r_{c,0}$ • r_0 • a • E • ν • ρ_s • X_{max}	• 11.2 W/(m·K) • 0.18 W/(m·K) • 0.531 • 1.4 • 10/9 • Not reported • Not reported • Not reported • Not reported • Not reported • 0.02075 µm • 2.5 µm • 0.5 • Not reported • Not reported • 7.44 g/cm3 • 1.40wt%	• 11.2 W/(m·K) • 0.18 W/(m·K) • 0.445 • 1.4 • 10/9 • Not reported • Not reported • Not reported • Not reported • Not reported • 0.0211 µm • 0.5 µm • 0.5 • Not reported • Not reported • 6.07 g/cm3 • 1.82wt%		193.15-413.15	10^{-4}-100
	k_{eff} ranges **(Exp. to model deviation < 35 %)**		• **Exp.** • **Model**	• **0.0313-1.25 W/(m·K)** • **0.0256-1.41 W/(m·K)**	• **0.566-1.36 W/(m·K)** • **0.755-1.45 W/(m·K)**			
				Bronze-water	Bronze-air	Aluminium-air	T (K)	P (bar)
3.1.8 Modified Zehner-Schlünder: area-contact model **[45]: AC**	• Glass • Stainless steel • Urea-formaldehyde • Bronze • Aluminium	• Water • Glycerol • Air	• ks • kg • C • m • ε • α	• 117 W/(m·K) • 0.623 W/(m·K) • 1.25 • 10/9 • 0.42 • 0.002	• 117 W/(m·K) • 0.0268 W/(m·K) • 1.25 • 10/9 • 0.42 • 0.002	• 218 W/(m·K) • 0.0268 W/(m·K) • 1.25 • 10/9 • 0.42 • 0.002	308.15	Not indicated
	k_{eff} ranges **(Exp. to model deviation < 35 %)**		• **Exp.**	• **4.61 W/(m·K)**	• **1.23 W/(m·K)**	• **3.89 W/(m·K)**		

			• **Model**	• **4.62 W/(m·K)**	• **1.50 W/(m·K)**	• **2.56 W/(m·K)**		
***3.1.9 Modified Zehner-Schlünder: phase-symmetry model* [45]: PS**	-	-	• ks • kg • B or ε	-			T (K)	P (bar)
				No comparison to experimental data			-	-
***3.1.10 Raghavan-Martin model* [49]: RM**	• $LaNi_{4.7}Al_{0.3}$ • HWT 5800	• H_2	• ks • kg • ε • A0 • A1	$LaNi_{4.7}Al_{0.3}$-H_2	HWT 5800-H_2		T (K)	P (bar)
				• 11.2 W/(m·K) • 0.18 W/(m·K) • 0.531 • 1/3 • 0.25	• 11.2 W/(m·K) • 0.18 W/(m·K) • 0.445 • 1/3 • 0.25		193.15-413.15	0.01-60
	k_{eff} ranges **(Exp. to model deviation < 2 %, expect at low ranges for for HWT 5800-H_2)**		• **Exp.** • **Model**	• **0.100-1.10 W/(m·K)** • **0.100-1.11 W/(m·K)**	• **0.167-1.07 W/(m·K)** • **0.101-1.09 W/(m·K)**			
***3.1.11 Improved area-contact model* [50]: IAC**	• $LaNi_5$	• H_2	• k_s • ε_0 • α_0 • B_0 • α_a • ϕ_p • ϕ_{abs}* • ϕ_{des}* • P_{eq} • R_P • d_0 • l • γ • a • μ • c_p	$LaNi_5$-H_2			T (K)	P (bar)
				• 8 W/(m·K) • 0.52 • Not reported • Not reported • ~0.03 (from a graph of α_a vs ϕ_{abs}) • 0.273 • 0.168 • 0.84 • From known PCI • ~13.3 (read from PCI at 333.15 K) • 15 μm • Not reported • Not reported • 0.3 • Not reported • Not reported			333.15	1-100
			* ϕ_{abs} and ϕ_{des} are given in place of V_0, V_1 and V_2, which can only be experimentally measured					
	k_{eff} ranges **(Exp. to model deviation < 15 %)**		• **Exp.** • **Model**	• **0.494-1.07 W/(m·K)** • **0.570-1.01 W/(m·K)**				
***3.1.12 Abdin-Webb-Gray model* [102]: AWC**	• $LaNi_5$ • $LaNi_{4.7}Al_{0.3}$	• H_2	• k_s • $k_{g,ref}$ • ε_0 • d_0 • d_v • C_1 • C_2 • E' • σ_R • Pr • α_{T1} • α_{T2} • γ	$LaNi_5$-H_2	$LaNi_{4.7}Al_{0.3}$-H_2**		T (K)	P (bar)
				• 2 W/(m·K) • 0.167 W/(m·K) • 0.5 • 12 μm • 29.37 μm • 7.3 GPa • -0.27 • Not reported • 0.12 μm • 0.6 • 0.69 • 0.83 • 1.4	• 12.5 W/(m·K) • 0.18 W/(m·K) • 0.531 • 5 μm • 31.11 μm • Not reported • Not reported • Not reported • Not reported • 0.6 • Not reported • Not reported • 1.4		293.15-303.55	0-10

			• b_g • P_{eq} • R_P • ϕ_p • ϕ_{abs}* • ϕ_{des}*	• 9.87 • An equation fitting exp. data is reported • Might be got from the same equation • 0.243 • 0.168 • 0.84	• 9.87 • Not reported • Not reported • Not reported • Not reported • Not reported		
			* ϕ_{abs} and ϕ_{des} are given in place of V_0, V_1 and V_2, which can only be experimentally measured ** It is said that parameters are taken from [98], but the most of them are not present and some are different				
	k_{eff} ranges **(Exp. to model deviation < 15 %, expect at low ranges for $LaNi_5$-H_2)**		• **Exp.** • **Model**	• **0.0433-1.93 W/(m·K)** • **0.159-1.78 W/(m·K)**	• **0.0577-1.06 W/(m·K)** • **0.0490-1.04 W/(m·K)**		
***3.1.13 Heat transfer concentrating model* [91]: HTC**				Not active $LaNi_{4.7}Al_{0.3}$-H_2	Not active HWT 5800-H_2	T (K)	P (bar)
	• Al_2O_3 • Steel • Si • SiC • Cr • Al • Fe • $LaNi_5$ • $LaNi_{4.7}Al_{0.3}$ (not active) • HWT 5800 (not active)	• Air • Ar • He • N_2 • H_2	• k_s • k_g • ε • d	• 12.5 W/(m·K) • 0.18 W/(m·K) • 0.531 • 6 μm	• 12 W/(m·K) • 0.18 W/(m·K) • 0.445 • 50 μm	293.15	10^{-5}-100
	k_{eff} ranges **(Exp. to model deviation < 22 %)**		• **Exp.** • **Model**	• **0.881 W/(m·K)** • **0.7758 W/(m·K)**	• **1.28 W/(m·K)** • **0.9945 W/(m·K)**		

Table S2. Experimental and model-calculated ETC values and parameters for different hydride forming and non-forming materials under different atmospheres, temperature and pressure conditions.

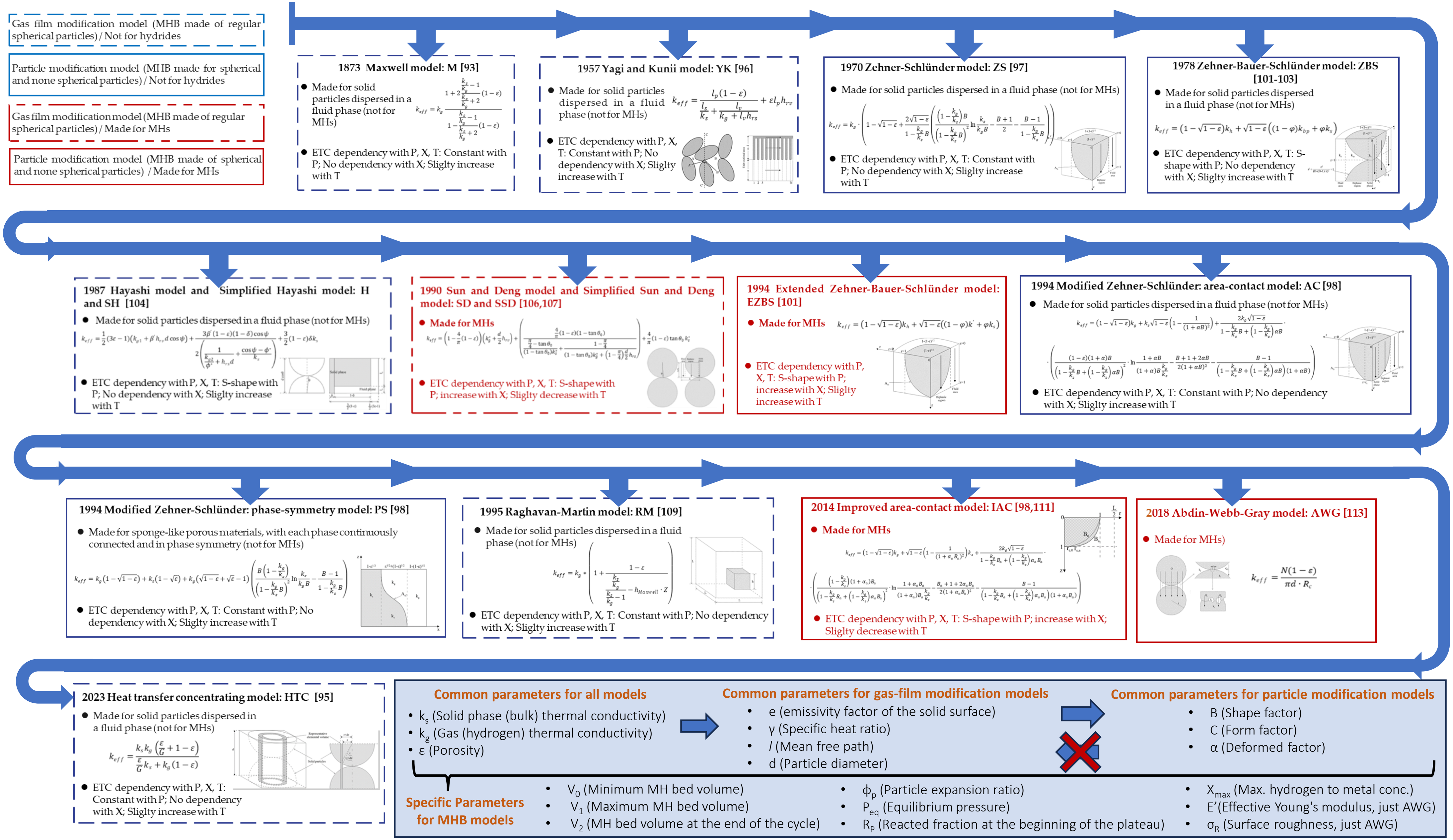

Figure S1. Summary of the ETC models: Classification, ETC dependence on P, T, and X, and common parameters.