

Supplementary Material for the Tutorial Review

**Recent advances in ex-ante techno-environmental-economic assessment of
thermochemical waste or biomass to energy technologies based on process simulation**

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Table S1 Coefficients for functions of equilibrium constants of reactions¹

Reaction	$\ln K = b_0 + b_1T + b_2T^{-1} + b_3\ln T + b_4T^2 + b_5T^{-2}$					
	b_0	b_1	b_2	b_3	b_4	b_5
$C + CO_2 \leftrightarrow 2CO$	25.655	-0.352×10^{-3}	-21574.471	-0.476	0	0.981×10^5
$C + H_2O \leftrightarrow CO + H_2$	7.643	-0.624×10^{-3}	-15702.009	1.384	0	0.399×10^5
$C + 2H_2 \leftrightarrow CH_4$	32.542	3.733×10^{-3}	7082.849	-6.567	-0.36×10^{-6}	-0.36×10^{-6}
$CO + H_2O \leftrightarrow CO_2 + H_2$	-18.014	-0.269×10^{-3}	5872.461	1.86	0	-58200
$CH_4 + H_2O \leftrightarrow CO + 3H_2$	-24.898	-4.354×10^{-3}	-22784.858	7.951	0.36×10^{-6}	4850

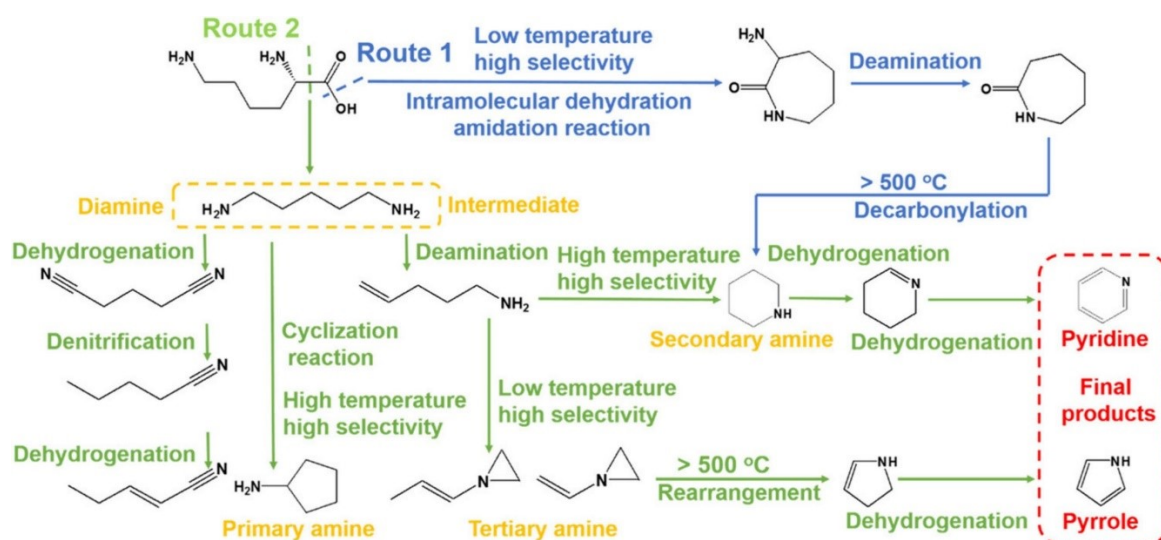


Fig. S2 Example of molecular-level mechanistic model (Reprinted with the permission.²

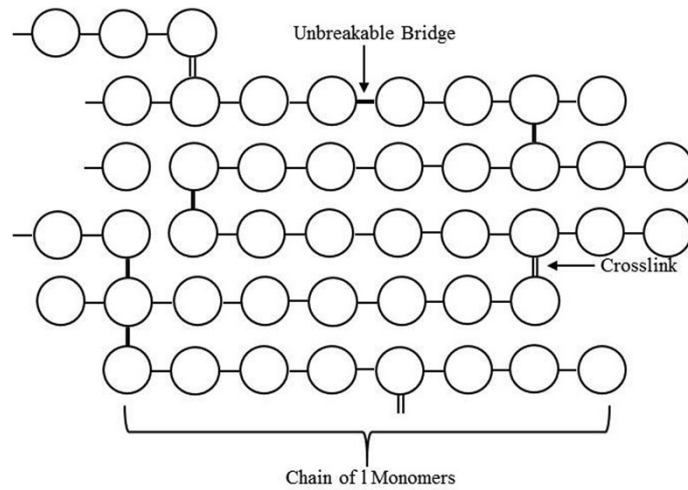


Fig. S3 Example of particle-level network model (Reprinted with the permission.³ Copyright 2019, 2020, and 2023, Elsevier Ltd)

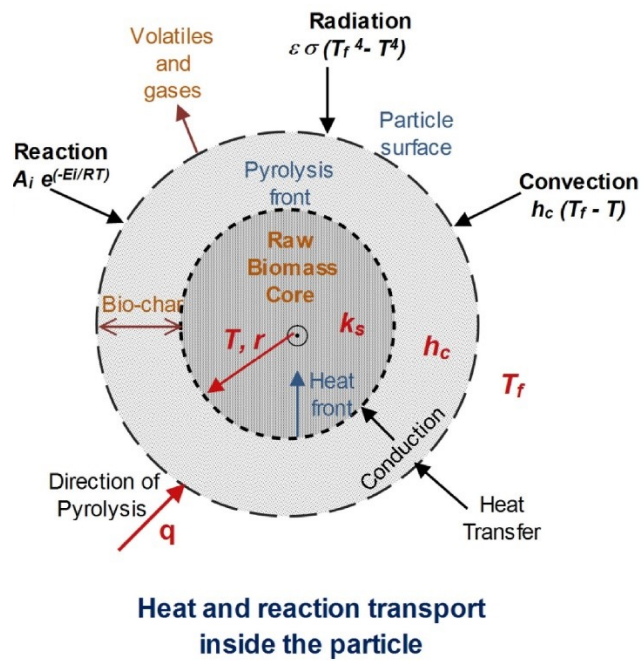


Fig. S4 Example of particle-level heat and mass transport model (Reprinted with the permission.⁴ Copyright 2019, 2020, and 2023, Elsevier Ltd)

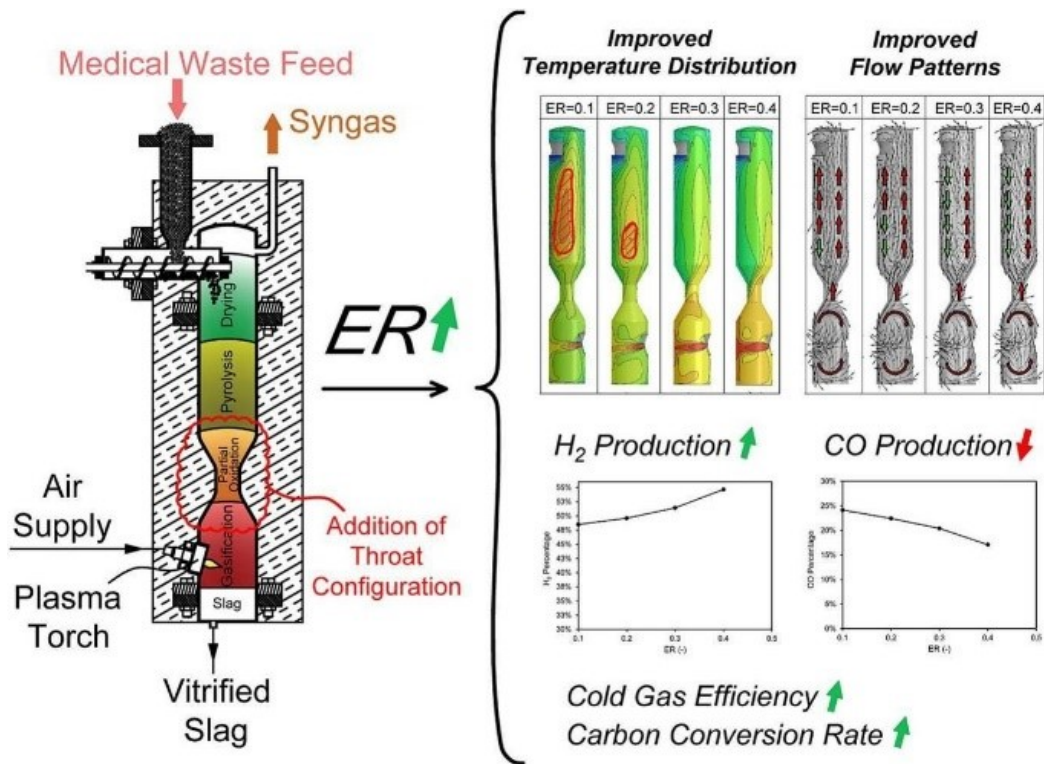


Fig. S5 Example of reactor-level CFD model (Reprinted with the permission.⁵ Copyright

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1. Moving grate reactor

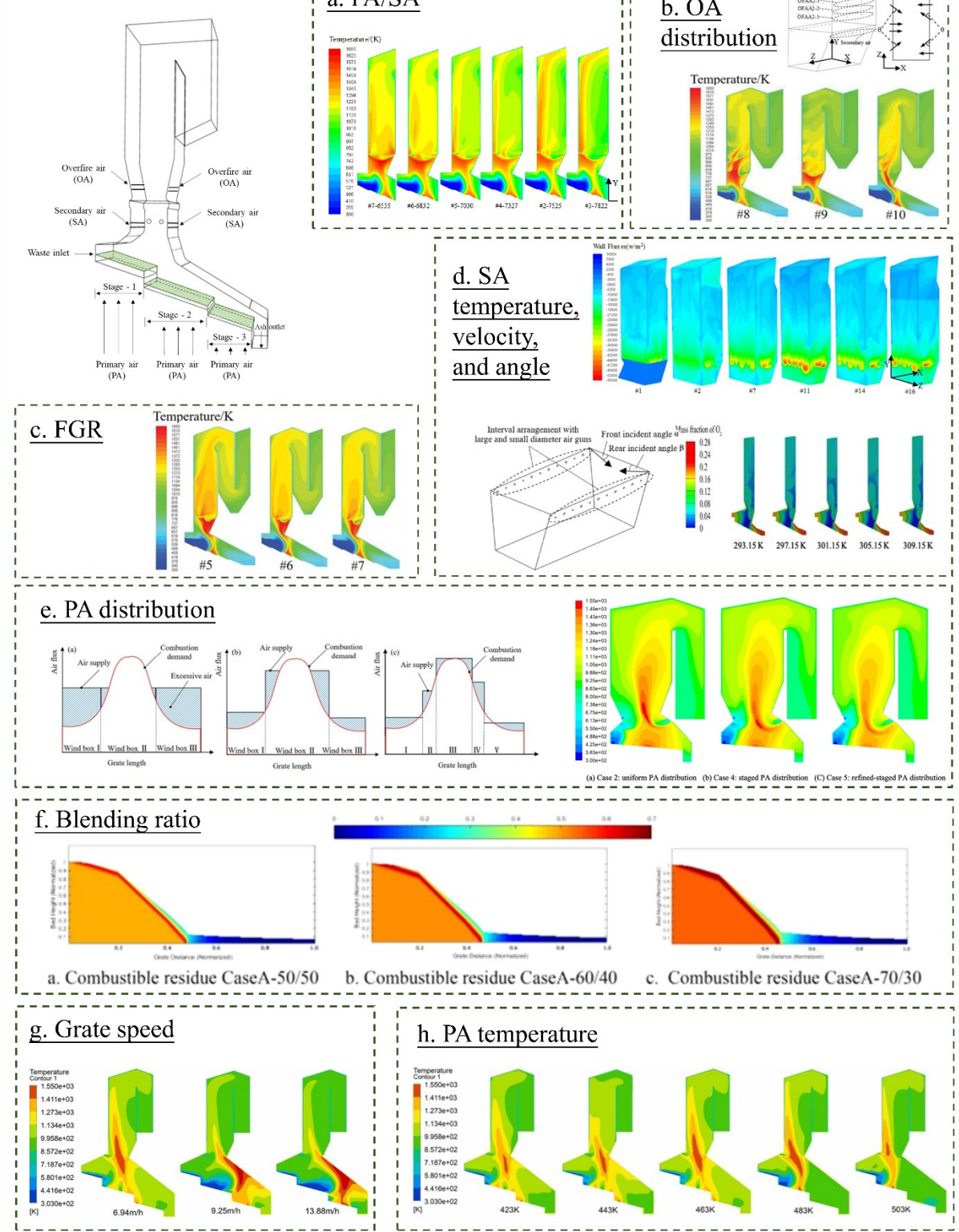


Fig. S6 Recent concentrations of local operational conditions in 1.moving grate reactor. Reprinted with the permission.⁶ Copyright 2024, Elsevier Ltd.. Effect of (a) PA/SA. Reprinted with the permission.⁷ Copyright 2022, Elsevier Ltd. (b) OA distribution. Reprinted with the permission.⁸

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(d) SA temperature, velocity, and angle. Reprinted with the permission.^{7,9} Copyright 2022 and 2024,
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Blending ratio. Reprinted with the permission.¹¹ Copyright 2020, Elsevier Ltd. (g) Grate speed.
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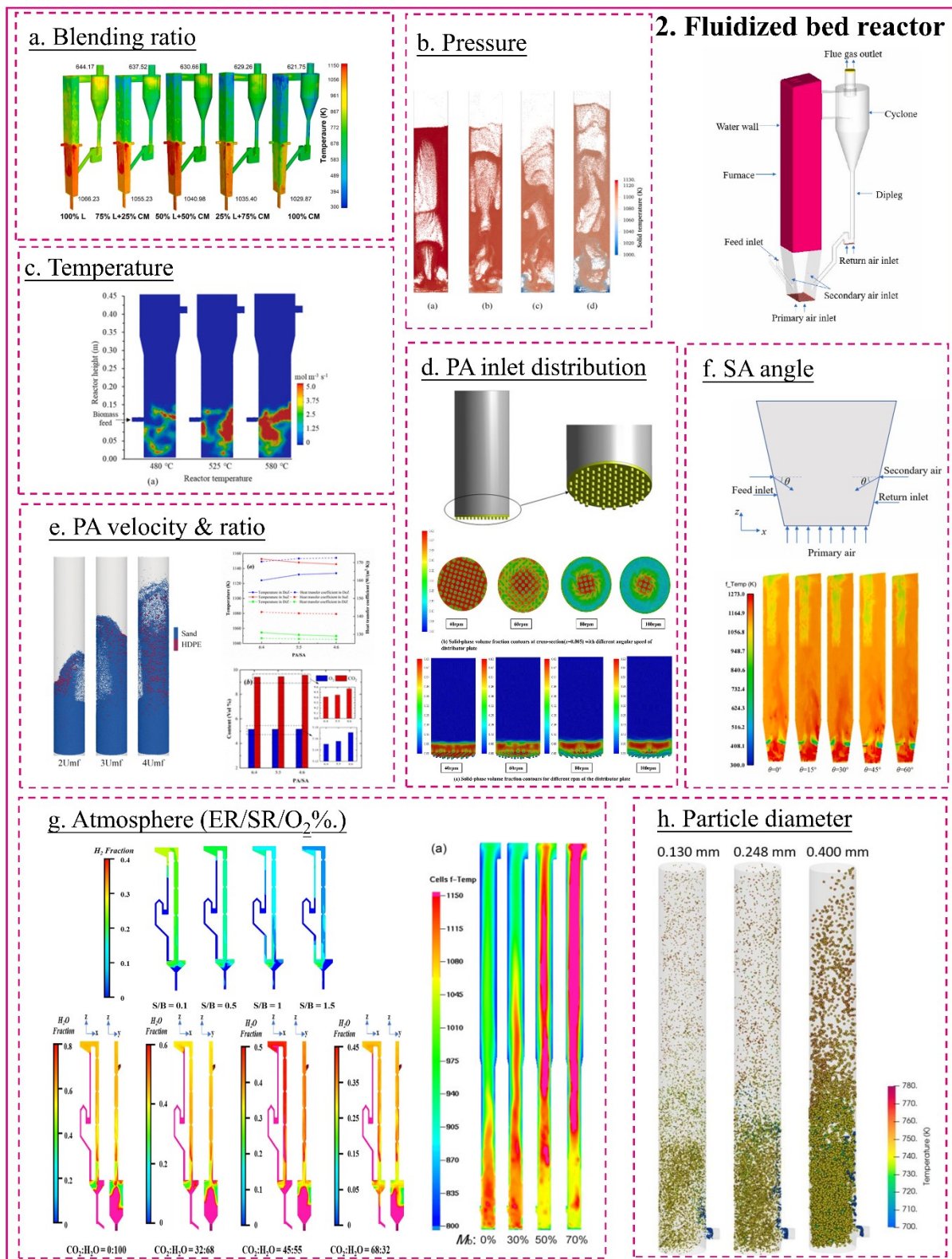


Fig. S7 Recent concentrations of local operational conditions in 2.fluidized bed reactor. Reprinted with

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PA inlet distribution. Reprinted with the permission.¹⁷ Copyright 2022, Elsevier Ltd. (e) PA velocity
& ratio. Reprinted with the permission.^{18, 19} Copyright 2021 and 2024, American Chemical Society. (f)

SA angle. Reprinted with the permission.¹³ Copyright 2024, Elsevier Ltd. (g) Atmosphere. Reprinted
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(h) Particle diameter. Reprinted with the permission.²² Copyright 2020, Elsevier Ltd.

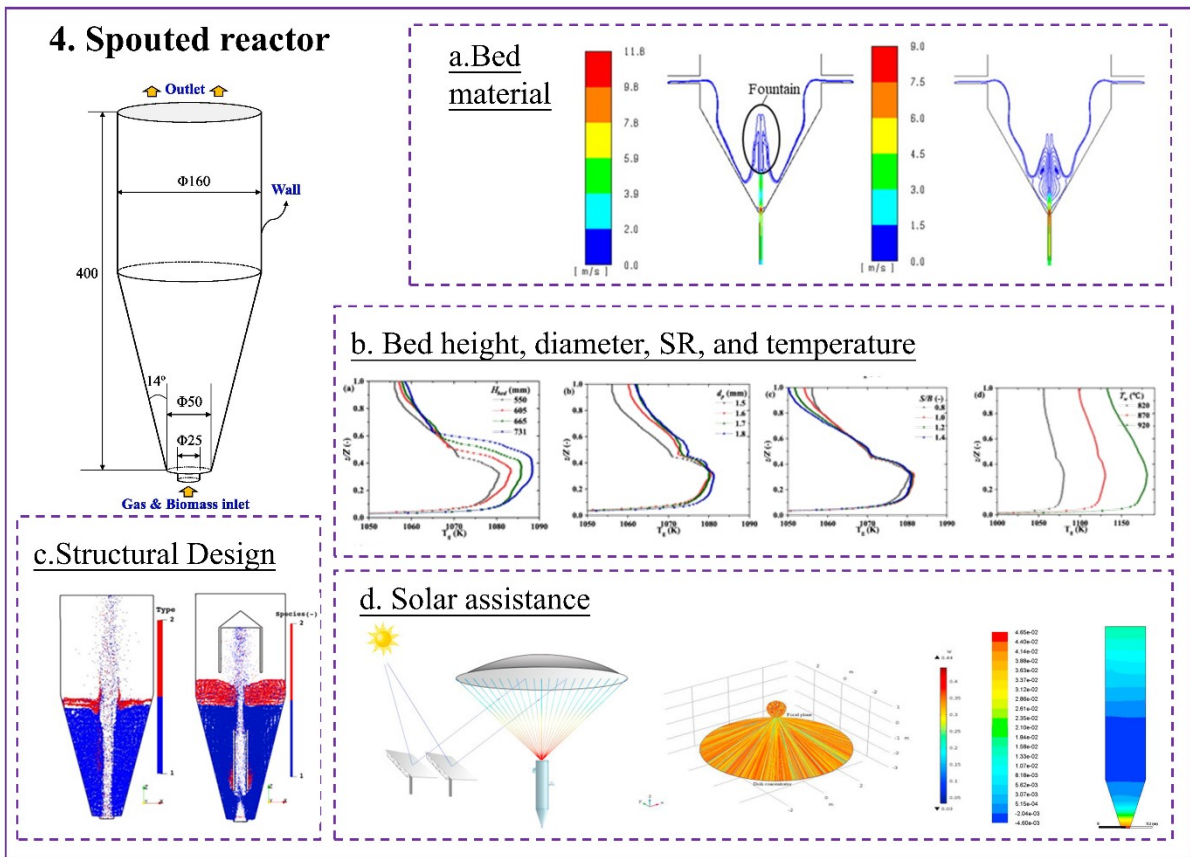
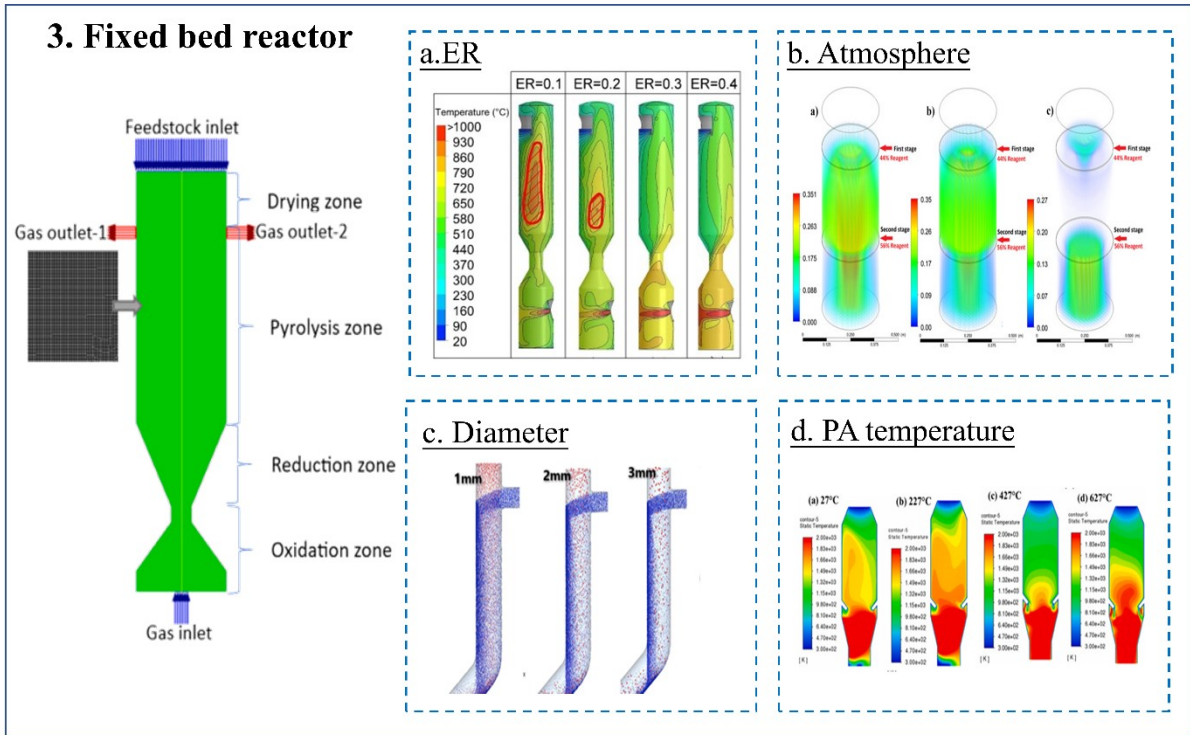


Fig. S8 Recent concentrations of local operational conditions in 3. fixed bed reactor and 4. spouted reactor. 3. Fixed bed reactor. Reprinted with the permission.²³ Copyright 2024, Elsevier Ltd. Effect of (a) ER. Reprinted with the permission.⁵ Copyright 2023, Elsevier Ltd. (b) Atmosphere. Reprinted with

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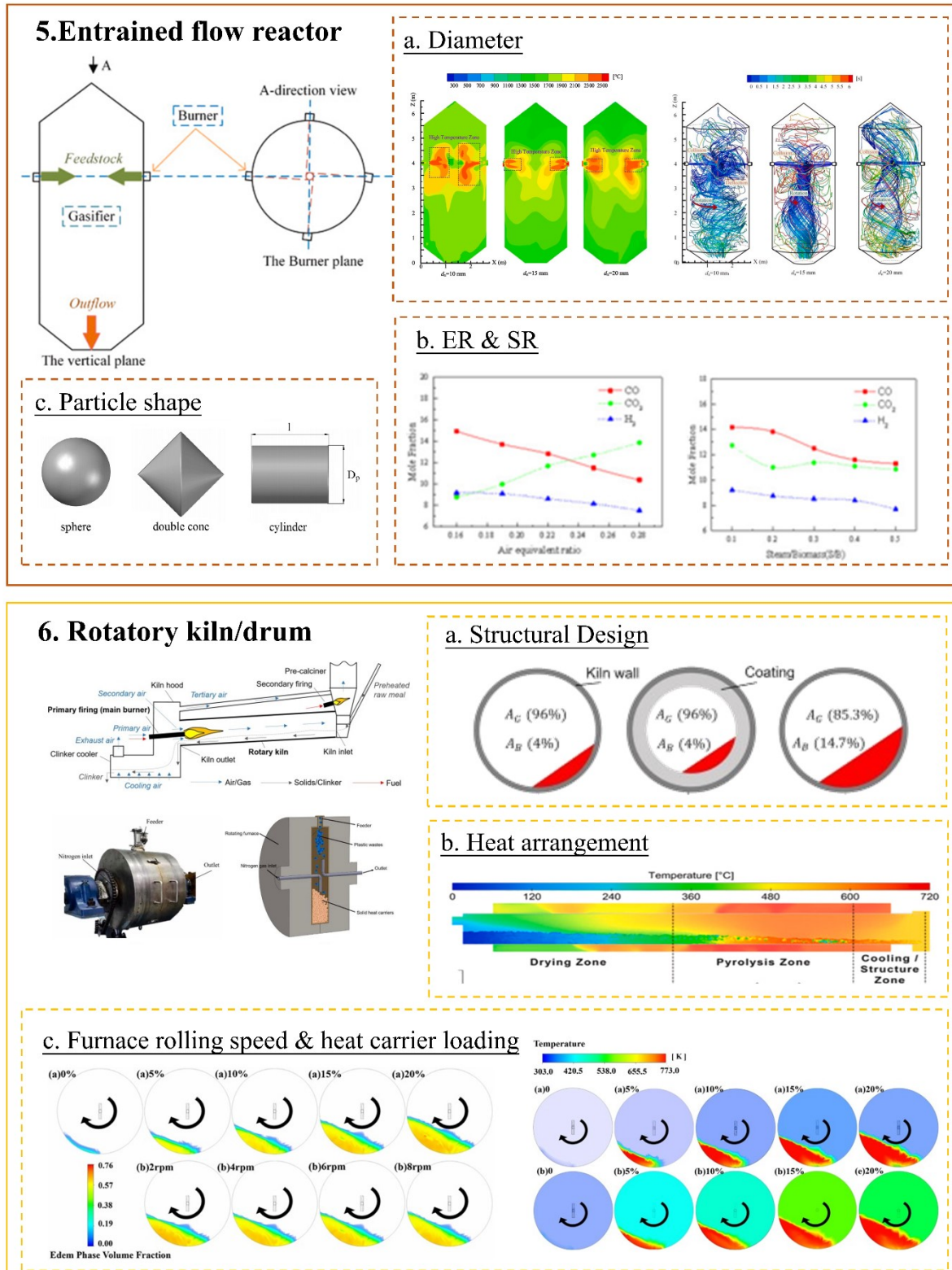


Fig. S9 Recent concentrations of local operational conditions in 5. 6ntrained flow reactor and 6. rotatory kiln/drum. (5) Entrained flow reactor. Reprinted with the permission.³² Copyright 2024, Elsevier Ltd. Effect of (a) Diameter. Reprinted with the permission.³² Copyright 2024, Elsevier Ltd. (b) ER and SR. Reprinted with the permission.³³ Copyright 2020, Elsevier Ltd. (c) Particle shape. Reprinted with the

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