Updates to OPGEE

OPGEE v3.0a candidate model

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CARB OPGEE Modeling update

California Air Resources Board

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energy resources engineering

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Outline

- Part 1: Background and context
- Part 2: Updates to the OPGEE model
  - Improving stream tracking
  - Gas processing simulation with process simulators
  - Gas fugitives modeling with improved datasets and statistical modeling
  - Gas functional unit allowed for primarily gas fields

Masnadi et al., Science, 361 (6405), 851-853.

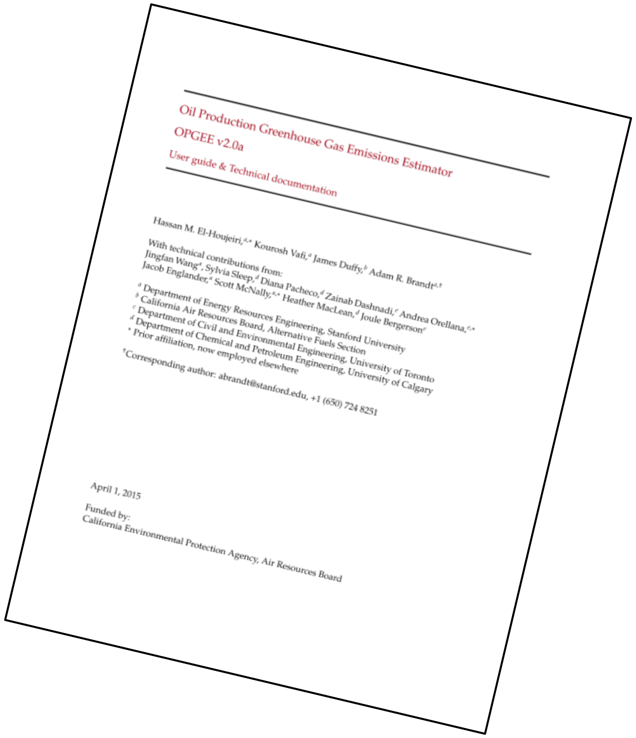
Part 1: Background and context

OPGEE model

- Model is called Oil Production Greenhouse gas Emissions **Estimator** (OPGEE)
- Estimates emissions given field parameters and technologies

The **first** open-source GHG tool for oil and gas operations

- Anyone can download, modify and use
- 36 published papers, complete documentation (~400 pp.) with all sources defined
- Funded by CARB, U.S. DOE, Carnegie Endowment, Ford Motor Co., Saudi Aramco



Oil Production Greenhouse Gas Emissions Estimator
OPGEE v2.0a
User guide & Technical documentation

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April 1, 2015

Funded by:
California Environmental Protection Agency, Air Resources Board

Source: El-Houjeiri and Brandt (2012a, 2012b)

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OPGEE model timeline

- Model development started in 2010
- First official version: OPGEE v1.0 released September 2012
- Second official version: OPGEE v2.0 released Feb 2018
- Third official version (candidate): OPGEE v3.0a - Introduced today

- Bibliography at end of slides:

Used in studies of crude oil CI for
- US (Cooney et al. 2017, Yeh et al 2017, Brandt et al. 2016)
- Canada (Cai et al. 2015, Englander et al. 2015)
- China (Masnadi et al. 2018a)
- Globe (Masnadi et al. 2018b)

Methods development
- Overall (El-Houjeri et al. 2013)
- Drilling (Vafi et al. 2016)
- Gas processing (Masnadi et al. 2020
- Uncertainty (Vafi et al. 2014a, 2014b, Brandt et al. 2015)
- Time trends (Masnadi et al. 2018c, Tripathi et al. 2017)

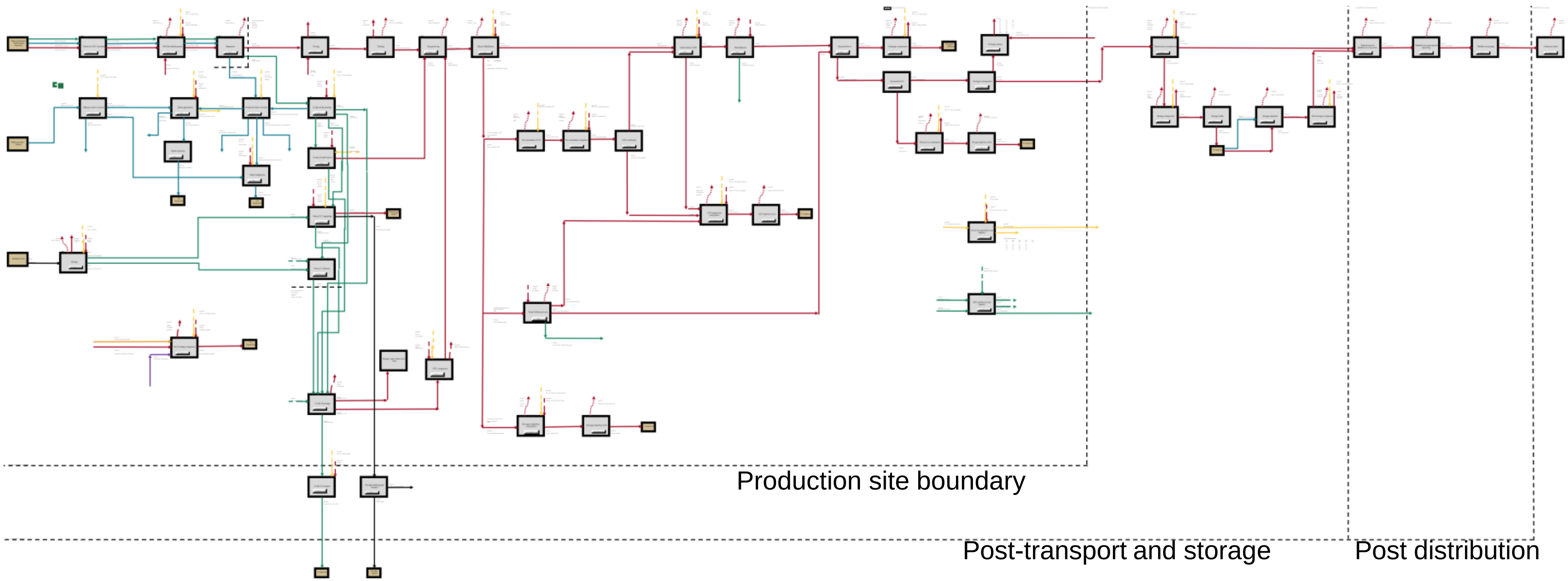
Part 2: Updates to the model

Challenge 1: Model organization and stream tracking

- OPGEE v2.0 had drawbacks in model organization and stream tracking
  - Gas balance sheet tracked gas species, but other streams were not reliably tracked
  - Process units were not on individual sheets, and unclear exactly which mass flows were entering and leaving each sheet
  - Pressures and other properties of streams not reliably tracked
  - No easy way to navigate along the processing path

- OPGEE v3.0a includes a completely reworked model "skeleton"
  - All streams of oil, water, gas, etc. are tracked in mass flows
  - Conservation of mass ensured at process unit and total model level
  - Pressures, temperatures, and other properties tracked
  - Navigation aided by graphical view of process connections (PFD)

Improvement: OPGEE 3.0 process flow sheet map



Streams differentiated by color

Green – Oil

Red – Gas

Blue – Water

Yellow – Electricity

Purple – Other gas

Black – Raw bitumen

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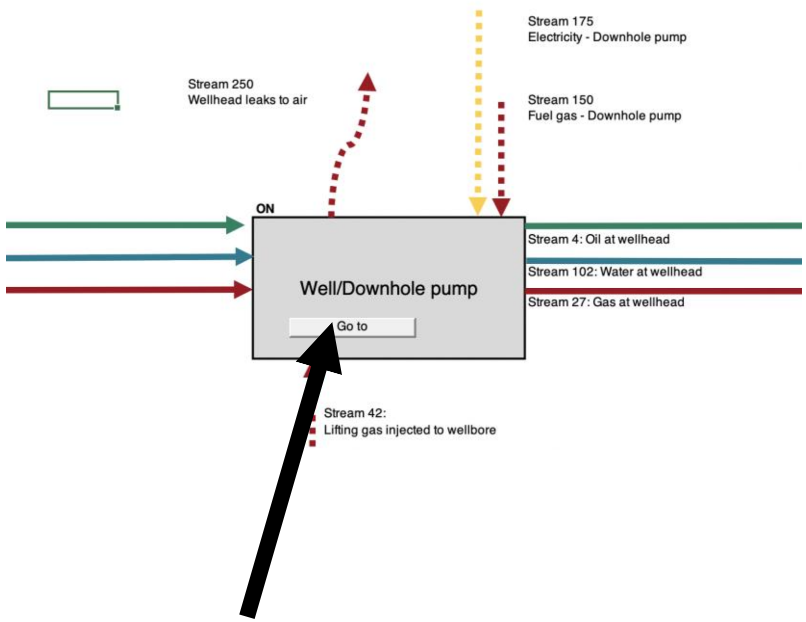
Graphical navigation



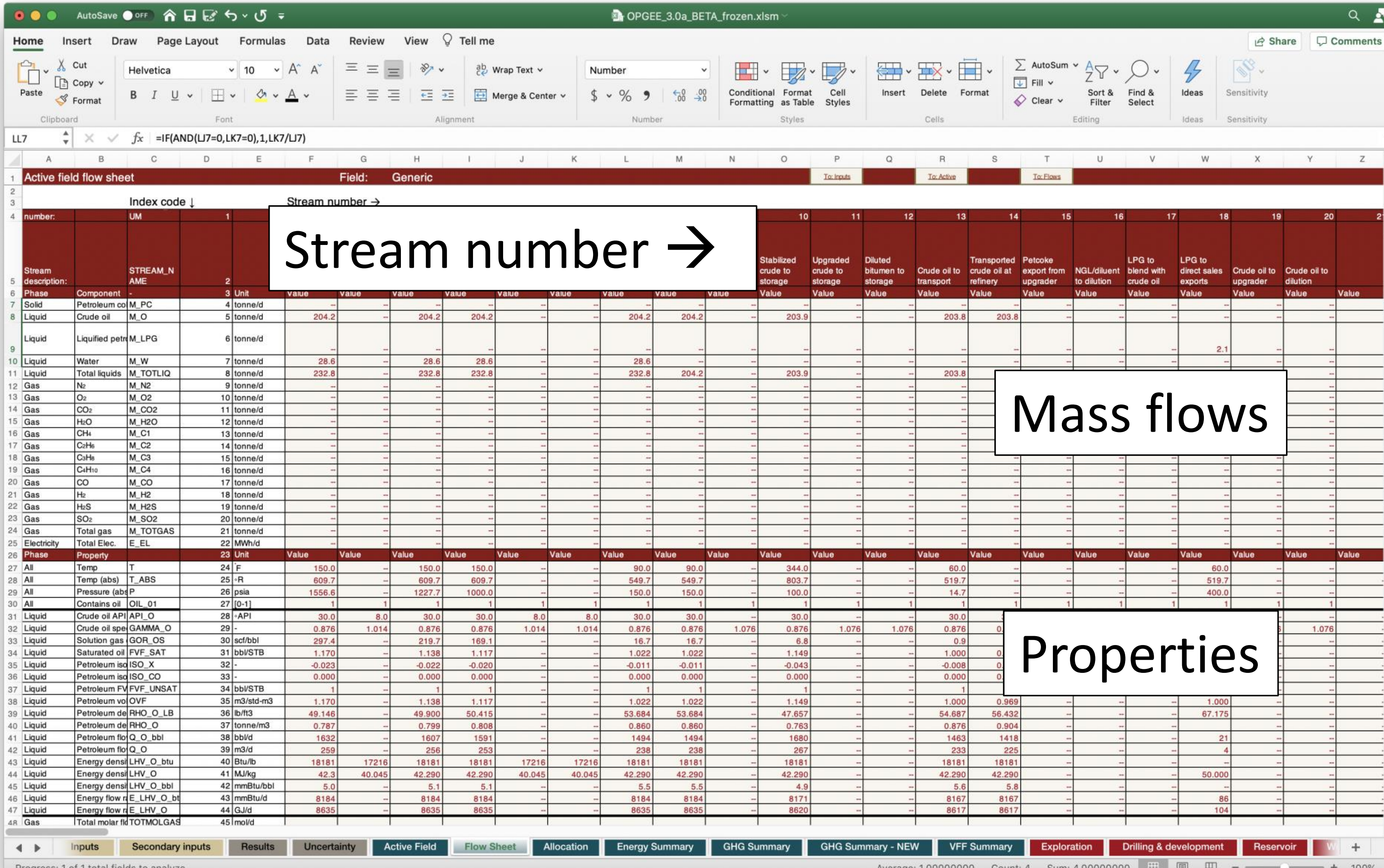
Trace flows along processing paths and click to navigate to sheets

Flows into process

STREAM_NUM	Stream number:			3	101	26	42
STREAM_NAME	Stream description:			Crude oil at well bottom	Water at well bottom	Gas at well bottom	Lifting gas to wellbore
-	Phase	Component	Unit	0	0	0	Value
M_PC	Solid	Petroleum co	tonne/d	–	–	–	--
M_O	Liquid	Crude oil	tonne/d	204.2	–	–	--
M_LPG	Liquid	Liquified petr	tonne/d	–	–	–	--
M_W	Liquid	Water	tonne/d	29	999	–	--
M_TOTLIQ	**Liquid**	**Total liq.**	**tonne/d**	233	999	–	--
M_N2	Gas	N_2	tonne/d	–	–	0.9	--
M_O2	Gas	O_2	tonne/d	–	–	–	--
M_CO2	Gas	CO_2	tonne/d	–	–	4.4	--
M_H2O	Gas	H_2O	tonne/d	–	–	–	--
M_C1	Gas	CH_4	tonne/d	–	–	22.5	--
M_C2	Gas	C_2H_6	tonne/d	–	–	2.0	--
M_C3	Gas	C_3H_8	tonne/d	–	–	1.5	--
M_C4	Gas	C_4H_{10}	tonne/d	–	–	1.0	--
M_CO	Gas	CO	tonne/d	–	–	–	--
M_H2	Gas	H_2	tonne/d	–	–	–	--
M_H2S	Gas	H_2S	tonne/d	–	–	0.6	--
M_SO2	Gas	SO_2	tonne/d	–	–	–	--
M_TOTGAS	Gas	Total gas	tonne/d	–	–	32.9	--
E_EL	Electricity	Total Elec.	MWh/d	–	–	–	--
-	Phase	Property	Unit	Value	Value	Value	Value
T	all	Temp	°F	150.0	150.0	150.0	150.0
P	all	Pressure	psia	1227.7	1227.7	1227.7	–
				Computed	Computed	Computed	From FT

Mass flows into and out of each process unit tracked

Flow sheet



OPGEE_3.0a_BETA_frozen.xlsm
Active field flow sheet
Field: Generic
Index code ↓
Stream number →
Stream number →
Mass flows
Properties

Mass balance tracking and error flagging

Errors easier to spot with mass balance tracking across entire model

	Inputs					Outputs						Totals			
	From production well	From makeup	From procesing stream	From rest of economy		Reinjected as water	Reinjected as steam	Disposed	-	Transport to market	To other stream	Total inputs	Total outputs	Ratio	
Petroleum coke			0.00					0.00	0.00	0	0.00	0	0	1.0000	OK
Unstabilized crude oil	17925			0.00					0.00	17828	97	17925	17925	[illegible]	OK
Natural gas liquids / Diluen			74.67	0.00					0.00	74.67	0.00	74.67	74.67	1.0000	OK
Water	37532	0				0	0	37532	0			37532	37532	1.0000	OK
	From well	From offsite	Imported fuel gas	stabilizer and tank	Upgrading proc. gas	Flared	Reinjected	Consumed	Vented and fugitives	Transport to market	To other stream	Total inputs	Total outputs	Ratio	
N_2	30.82	0.00	0.00	0.00	0.00	3.52	21.63	4.61	1.07	0.00	0.00	30.82	30.82	1.000000	OK
O_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.000000	OK
CO_2	145.27	0.00	0.00	0.64	0.00	16.59	0.00	0.00	2.44	0.00	126.88	145.91	145.91	1.000000	OK
H_2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.000000	OK
CH_4	741.28	0.00	0.00	85.28	0.00	84.67	530.71	113.03	97.28	0.00	0.88	826.57	826.57	1.000000	OK
C_2H_6	66.16	0.00	0.00	5.72	0.00	7.56	6.64	1.41	1.31	54.97	0.00	71.89	71.89	1.000000	OK
C_3H_8	48.51	0.00	0.00	3.18	0.00	5.54	0.79	0.17	0.85	0.00	44.35	51.69	51.69	1.000000	OK
C_4H_{10}	31.97	0.00	0.00	1.91	0.00	3.65	0.19	0.04	0.55	0.00	29.45	33.88	33.88	1.000000	OK
CO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.000000	OK
H_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.000000	OK
H_2S	18.75	0.00	0.00	0.00	0.00	2.14	0.00	0.00	0.31	0.00	16.29	18.75	18.75	1.000000	OK
SO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.000000	OK
Total	1082.77	0.00	0.00	96.73	0.00	123.67	559.96	119.26	103.80	54.97	217.84	1179.50	1179.50	1.000000	OK
														Overall	OK

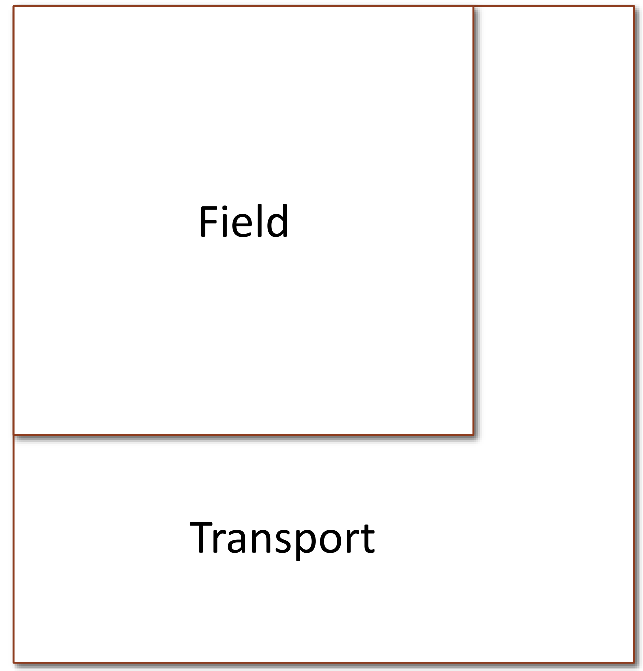
Gas as a primary product, different assessment points

OPGEE 2.0 always required oil to be the primary product

CI: gCO_2/MJ **oil** at refinery inlet

OPGEE 3.0 allows for gas as the primary product

CI: gCO_2/MJ **gas** at transportation system inlet



Oil at field boundary or refinery inlet

Gas at field boundary, transportation inlet or consumer

Challenge 2: Gas processing simulation

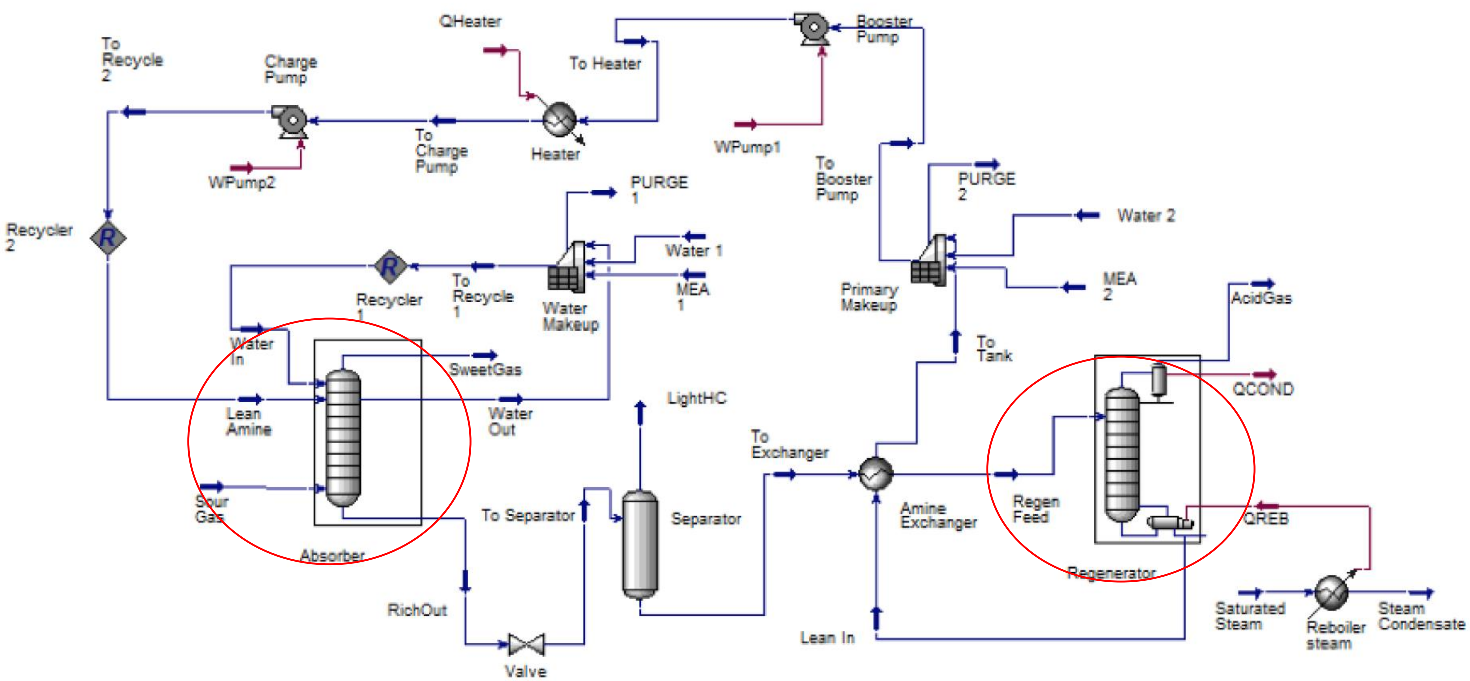
- OPGEE v2.0 had relied on ”textbook” treatment of gas processing units
  - Models largely taken from classic text Manning and Thompson
  - Simple models of energy use and power requirements per unit of throughput
  - No way to customize process unit energy use for particular conditions
  - Feedback from industry: “Why not use process simulation tools?”

- OPGEE v3.0a includes ”proxy” models generated from process simulation tools
  - Obtained access to Aspen HYSYS process simulation package
  - Work from template models of 4 key gas processing units
    - Acid Gas Removal, Dehydration, Demethanizer, Claus Unit
  - Simulated many cases at a variety of conditions
  - Generated statistical representations to predict Aspen HYSYS results

M.S. Masnadi *, P.R. Perrier , J. Wang , J. Rutherford , A.R. Brandt.
Statistical proxy modeling for life cycle assessment and energetic analysis.
Energy DOI: 10.1016/j.energy.2019.116882

Example: AGR modeling using process simulation software

- Modeled AGR unit in Aspen HYSYS chemical process simulation
- Five different solvents (amines):
  - 1. MEA; 2. DEA (30% wt.); 3. DEA high load (35% wt.); 4. MDEA; 5. DGA
- Five independent variables:
  - 1. CO_2 concentration; 2. H_2S concentration; 3. Regeneration reflux ratio; 4. Regeneration feed temperature; 5. Acid gas pressure



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Sampling approaches

AGR input variables to be sampled:

CO_2 concentration in gas

H_2S concentration in gas

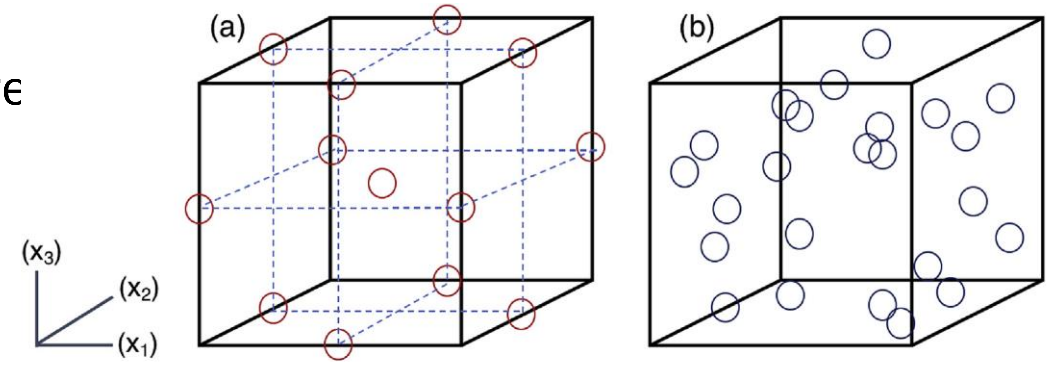
Reflux ratio

Regenerator feed temperature

Feed gas pressure

Deterministic sampling:
Box-Behnken

Random sampling:
Latin hypercube



Total of **~9000 simulations** of AGR systems across independent variables

Proxy modeling (cont'd)

- Experimental design: five independent variables
  - Settings of each dependent on type of solvent applied
  - Model is allowed to adjust some parameters to make simulation converge (e.g., amine circulation rate)
  - Save combination of 5 input variables plus multiple outputs

Variable	MEA	DGA	DEA	DEA-HL	MDEA
Reflux ratio [-]	1.5 – 3.0	1.5 – 3.0	1.5 – 3.0	1.5 – 3.0	6.5 – 8.0
Regen. feed temp. [°F]	190 – 220	190 – 220	190 – 220	190 – 220	190 – 220
Feed gas pressure [psia]	14.7 – 514.7	14.7 – 514.7	14.7 – 514.7	14.7 – 514.7	14.7 – 514.7
Amine loading [wt.%]	20	60	30	35	50
Amine circ. rate[a]	Var.	Var.	Var.	Var.	Var.
H_2S conc. [mol.%]	1 – 20	1 – 20	1 – 20	1 – 20	1 – 20
CO_2 conc. [mol.%]	1 – 15	1 – 15	1 – 15	1 – 15	1 – 15

Training and testing dataset

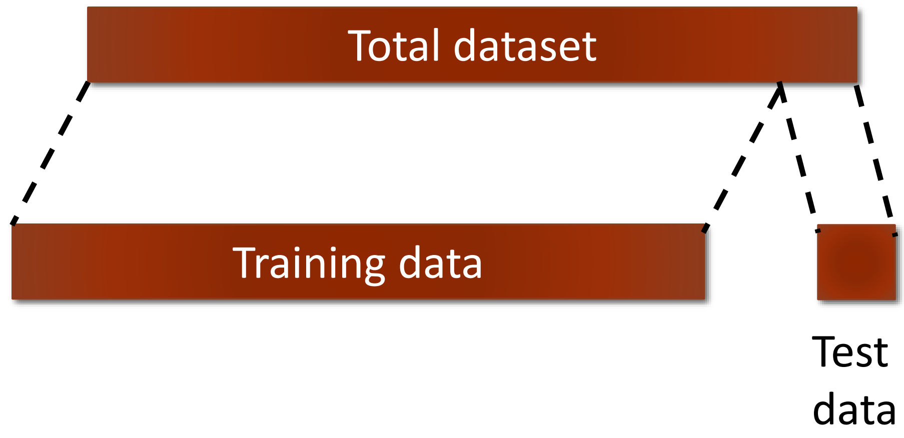
After 9,000 simulations, dataset is split into training and testing

Training data used to fit optimal model functional form

Test data “held out” and never examined until reporting results

Tested variety of polynomial and other classical models

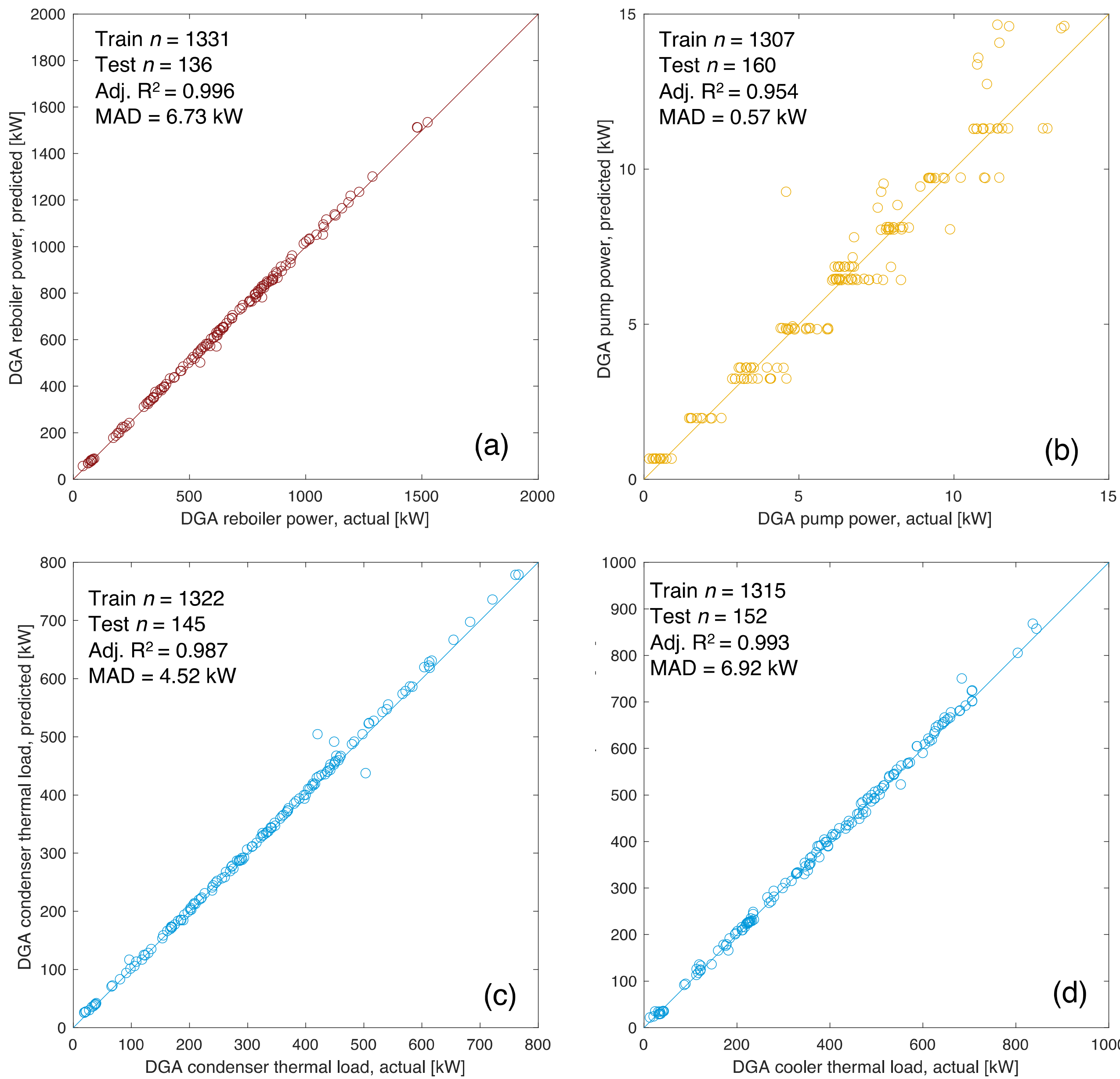
Quadratic regression balances complexity and fit



90% training
10% testing

$$P = \beta_0 + \sum_{i=1}^{5} \beta_a x_i + \sum_{i=1}^{5} \sum_{j=i+1}^{5} \beta_b \left(x_i \times x_j \right) + \sum_{i=1}^{5} \beta_c x_i^2$$

Test fitted AGR model against hold-out set



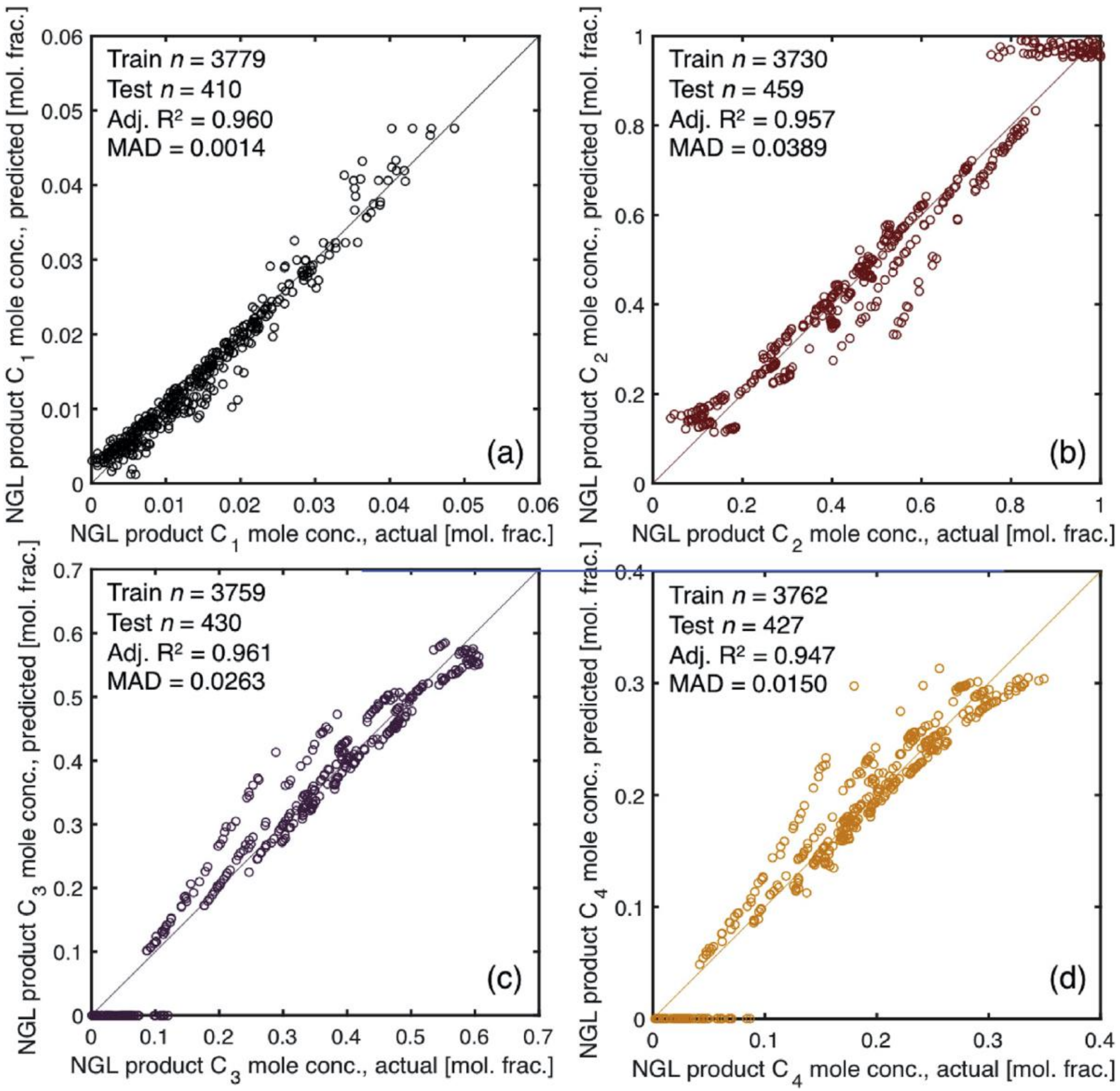
Reboiler

Pump

Condenser

Cooler

Demethanizer product composition results



Composition and shares of C1, C2, C3 to streams harder to predict

Take-aways from process simulation

- Quadratic regression able to fit extremely well in most cases
- Most fits have $R^2 > 0.95$
- OPGEE now produces, for cases within our sampled input ranges, results very close to Aspen HYSYS

<u>Challenges for extension</u>

Expertise and software license

Computational requirements very large for 10,000s of simulations

Unable to extrapolate – Can only model ranges of T, P, composition sampled

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Challenge 3: Fugitive and vented CH_4 emissions

- OPGEE v2.0 relied on CARB survey data for fugitive and vented CH4
  - Survey of California producers required detailed reporting on emissions
  - Emissions factors obtained from EPA GHG Inventory
  - Survey unable to account for differences between US regions
  - Independent measurements lacking, with lots of studies done since OPGEE v2.0

- OPGEE v3.0a includes modern, independently measured field data for CH_4 emissions sources
  - Two models: “site” and “component” level
  - Component level data draws from multiple studies, 1000s of measured leaks
  - Monte Carlo sampling approach includes super-emitter characteristics
  - Able to recreate observed US wide emissions (e.g., Alvarez et al. 2018)

J.S. Rutherford, E.D. Sherwin, A.P. Ravikumar, G.A. Heath, J.G. Englander, D. Cooley, D. Lyon, M. Omara, Q. Langfitt, A.R. Brandt Closing the gap: Explaining persistent underestimation by US oil and natural gas production-segment methane inventories Submitted: Nature Energy

Different varieties of methane measurement inform our understanding of emissions quantities and sources

Bottom-up

Component-level

e.g., EPA Greenhouse Gas Inventory

Site-level

e.g., Alvarez et al. 2018, National estimate

Top-down

e.g., Zhang et al. 2020, Permian Basin

Policy and programs

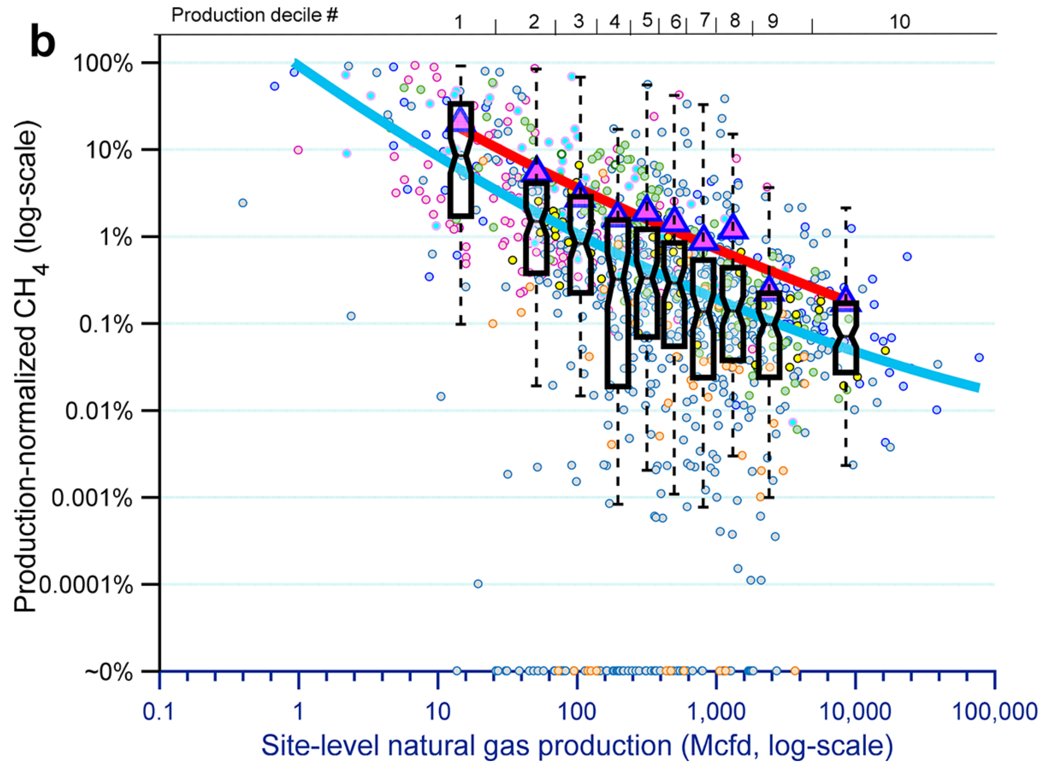
Validation and assessment

Site-level emissions for production operations

Site level loss rates can be assessed from downwind or above-view measurements

About 1000 sites from many basins compiled in Omara 2018

Relationship between production rate and loss rate imported and used to estimate site-level emissions



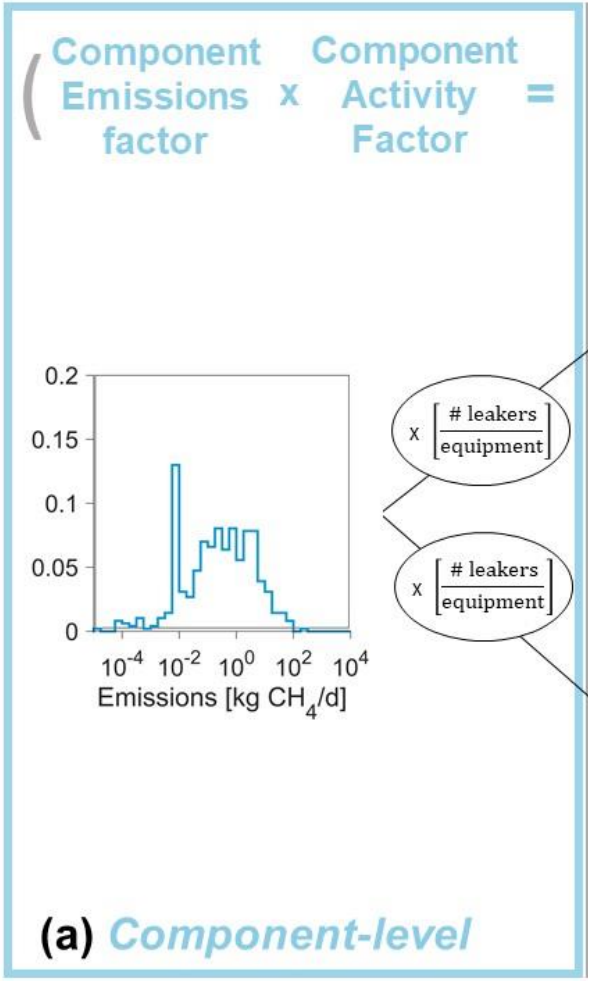
Source: Omara 2018

Collecting component-level data from various studies

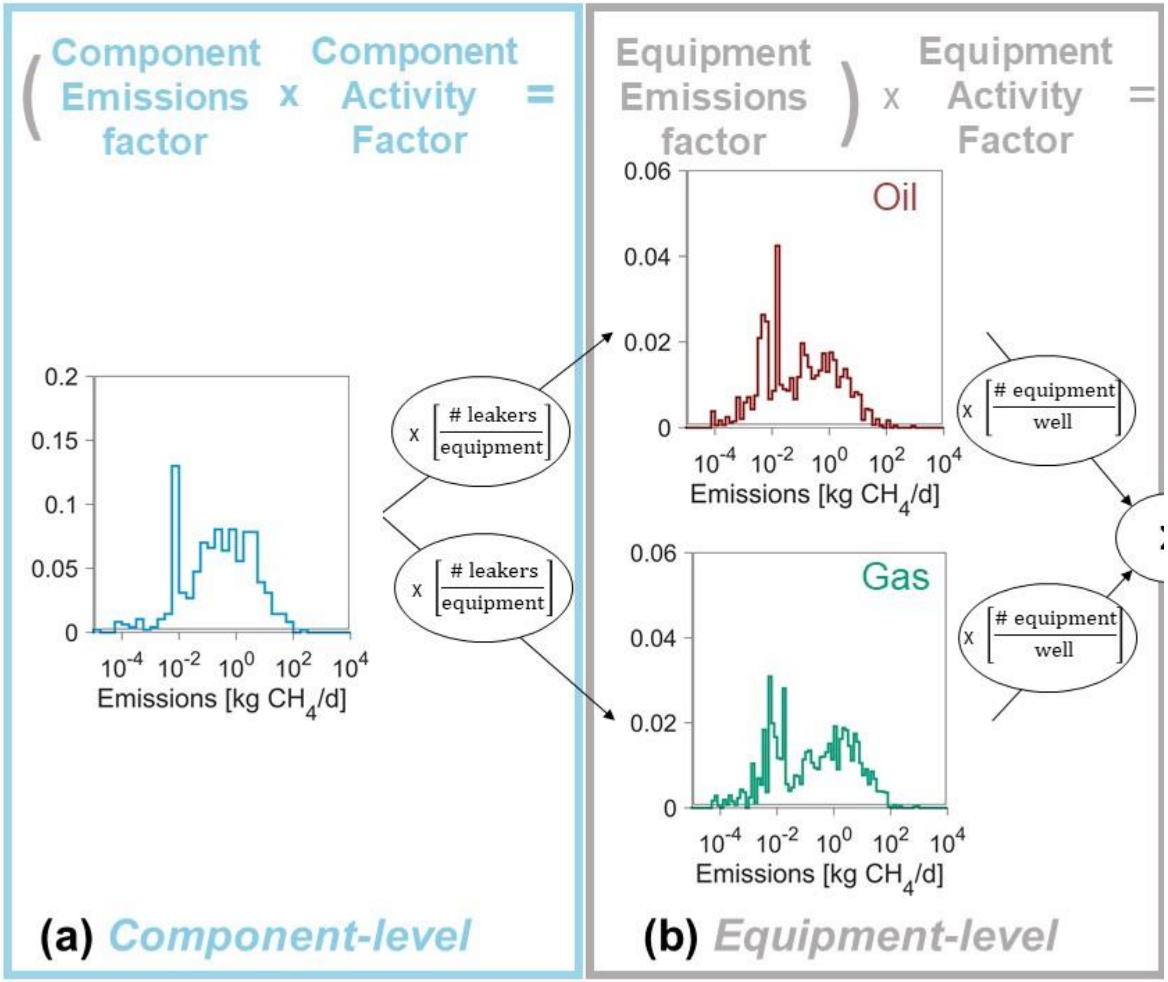
- Informed by comprehensive literature search of component-level surveys (6 studies, ~3200 measurements)
- Filtered to (in current OPGEE version) include US studies only
  - Limited global coverage
  - Future model versions could include emissions distributions from other regions

- Data consolidated to consistent component and equipment type categories
  - Consistent component definitions (details in full paper) allow combination of samples from different studies
  - Consistent equipment definitions allows generation of component counts per equipment

Development of a bottom-up tool



Development of a bottom-up tool



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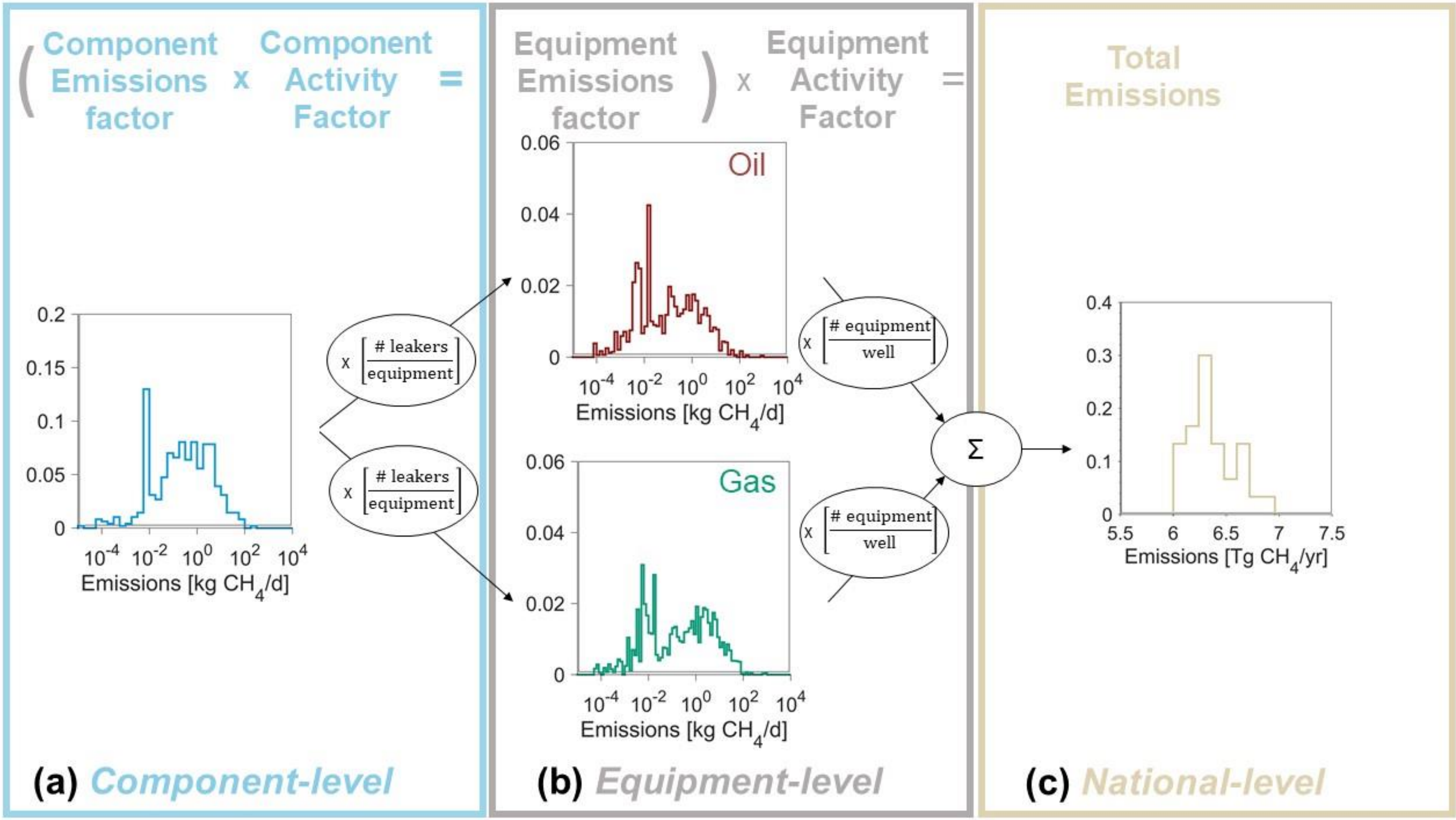
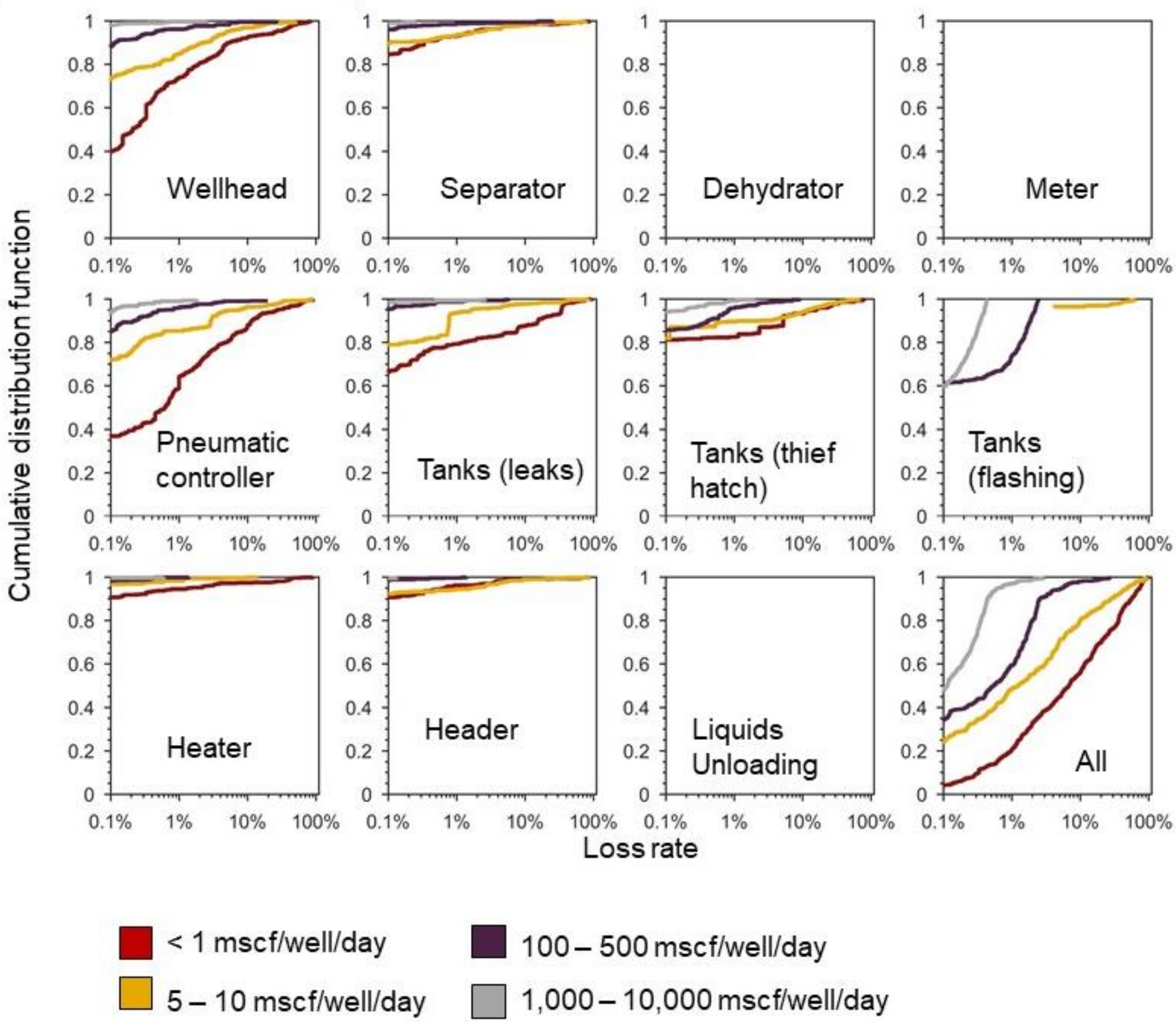
Development of a bottom-up tool



Fraction loss rates: Oil wells (<100 mscf/bbl)



Results of loss fraction are strong function of well productivity

This effect has been seen repeatedly in the empirical literature

Using equipment distributions in OPGEE

- A separate equipment-level loss fraction distribution is generated for each productivity tranche
  - A stochastic leak process will tend to cause higher loss fraction in less productive wells, even if that well is same age or has similar equipment type

- Resulting equipment distributions can be used in two ways in OPGEE
  1. Deterministic: Create average equipment leakage rate for a given productivity tranche
  2. Uncertainty: Draw a given number of equipment realizations for the size of the population you are analyzing, randomized from the sampled equipment types

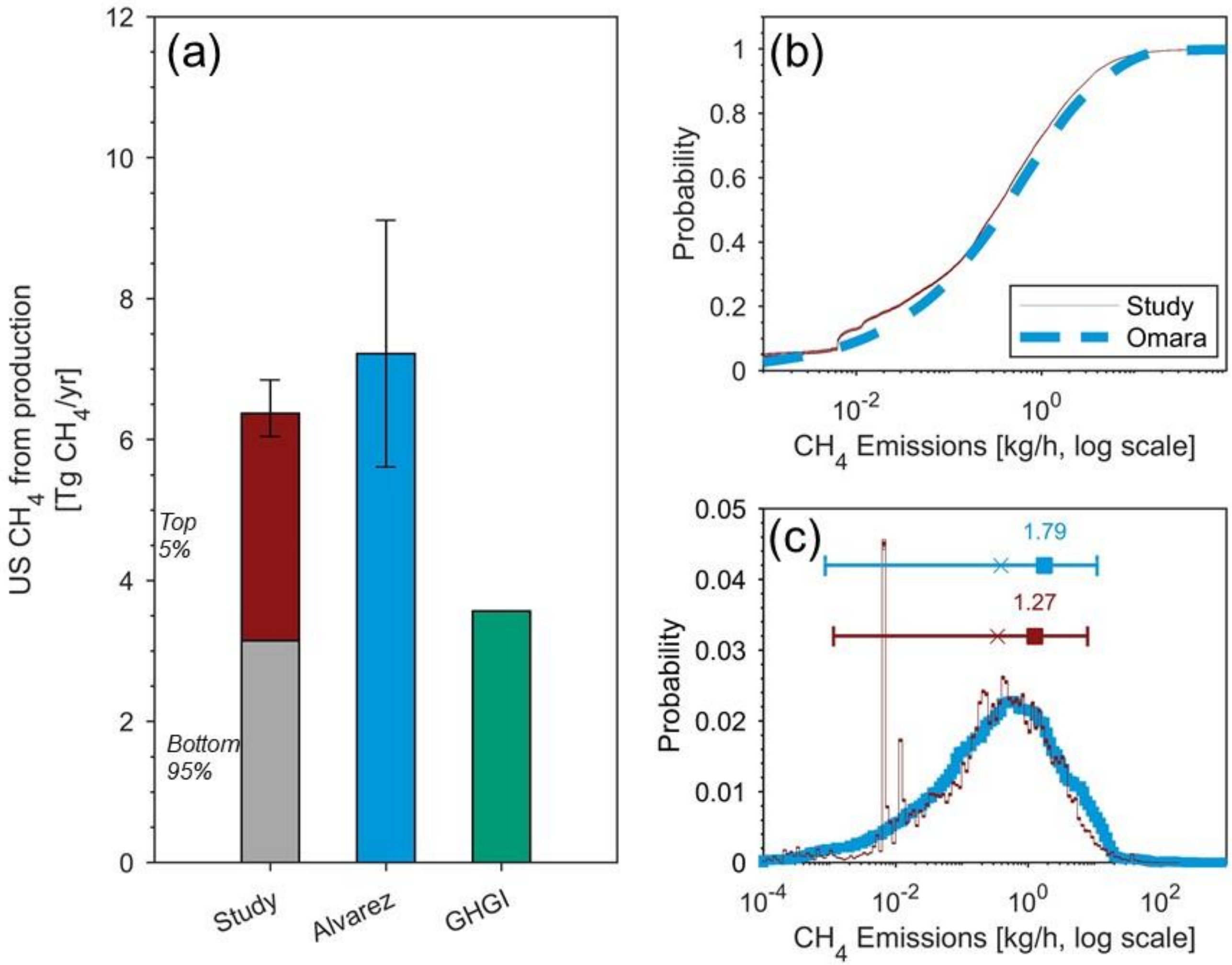
Validating the method

Ideally the method adopted in OPGEE would recreate the key results of the literature on methane emissions from the last 5 years

Key empirical features that have been found repeatedly that any tool should be able to show:

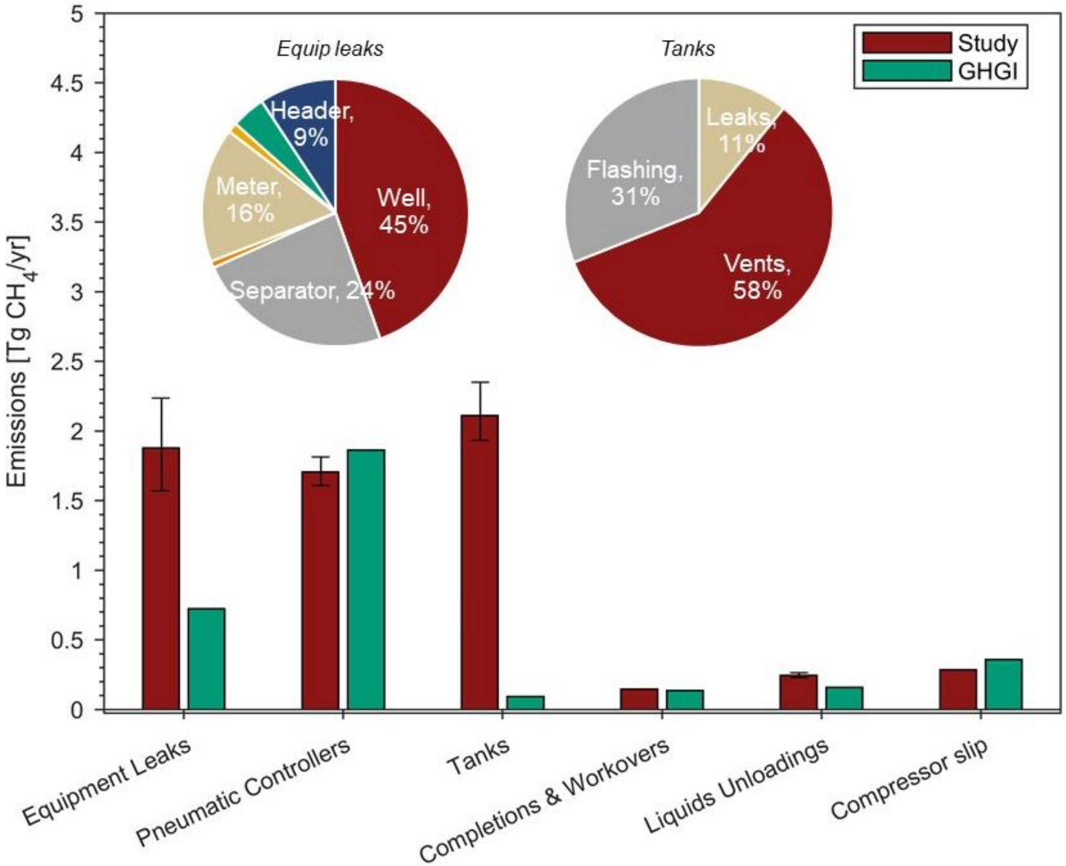
1. Larger emissions than classical EPA Greenhouse Gas Inventory methods
2. Strong dependence of loss fraction on site productivity
3. Strong "heavy-tailed" behavior of emissions distributions: dependence on large emitters to drive large fraction of emissions

Validating against US estimate of production-segment emissions



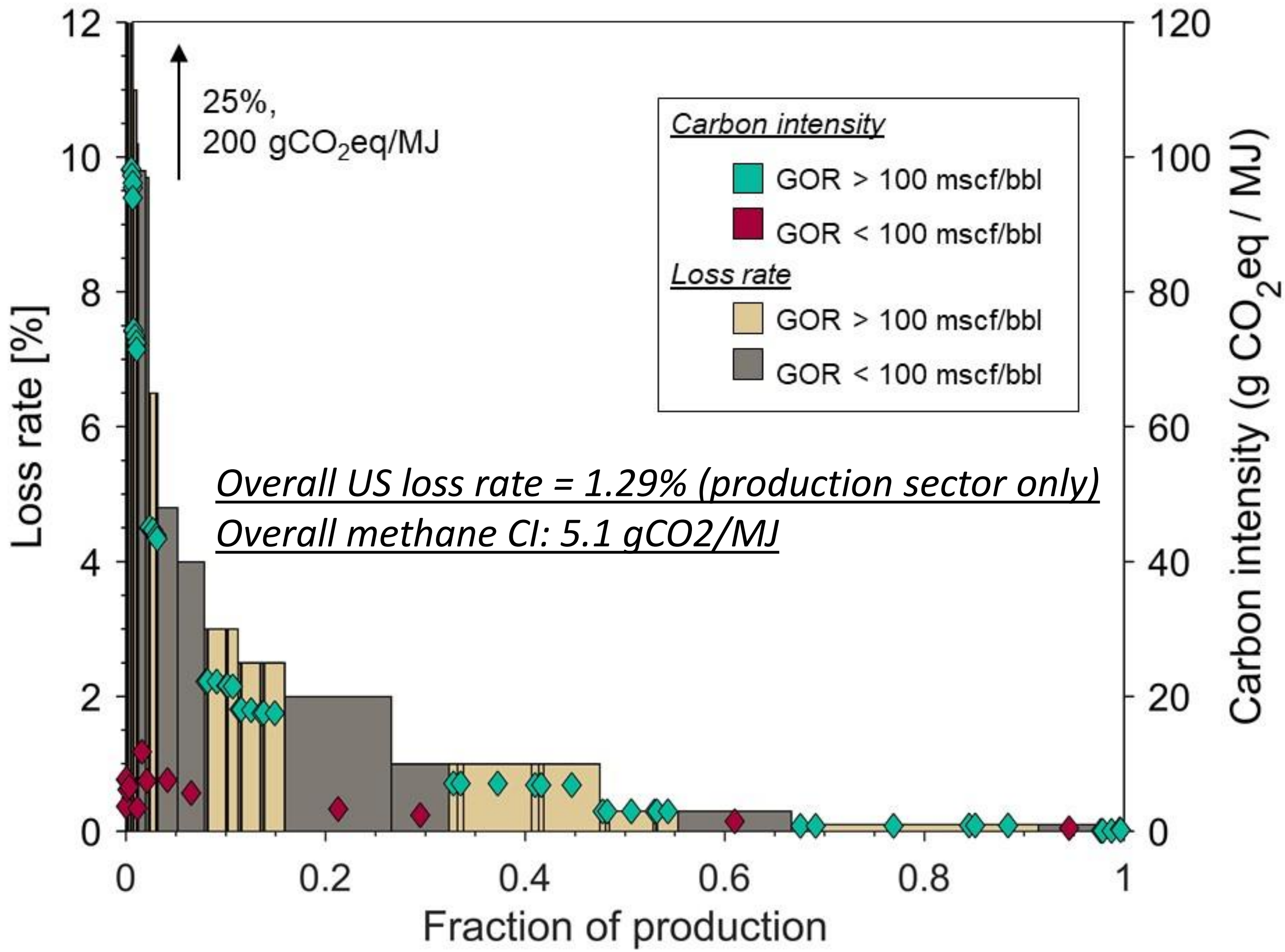
- Total emissions: Alvarez et al. 2018
- Probability distributions: Omara et al. 2018

US estimate of production-segment emissions by source



- Largest discrepancies between US EPA Greenhouse Gas Inventory and our results:
  - (2.1 Tg CH_4) Tank flashing and venting emissions
  - (1.4 Tg CH_4) Equipment leaks

Results for the upstream US oil and gas sector



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