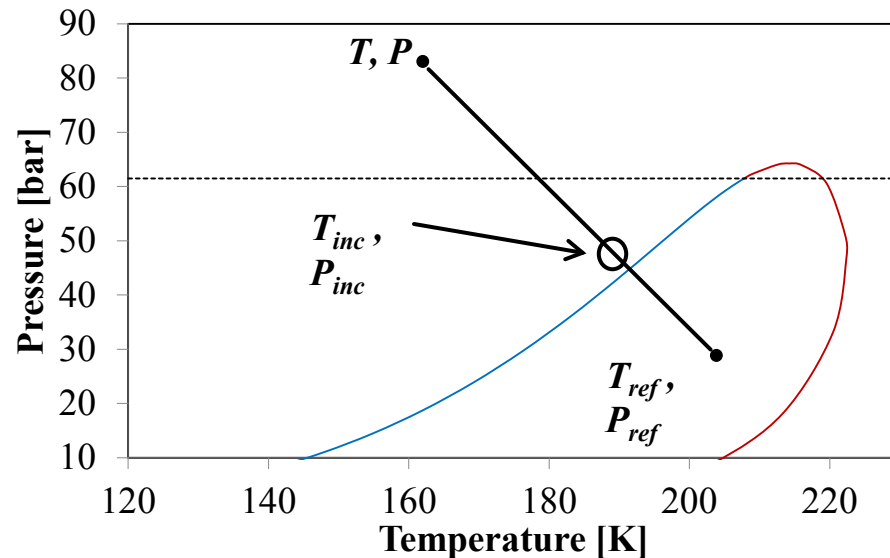


Time-efficient integration of the thermodynamics in heat-exchanger modelling

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2'nd Trondheim Gas Technology Conference November 2-3 2011

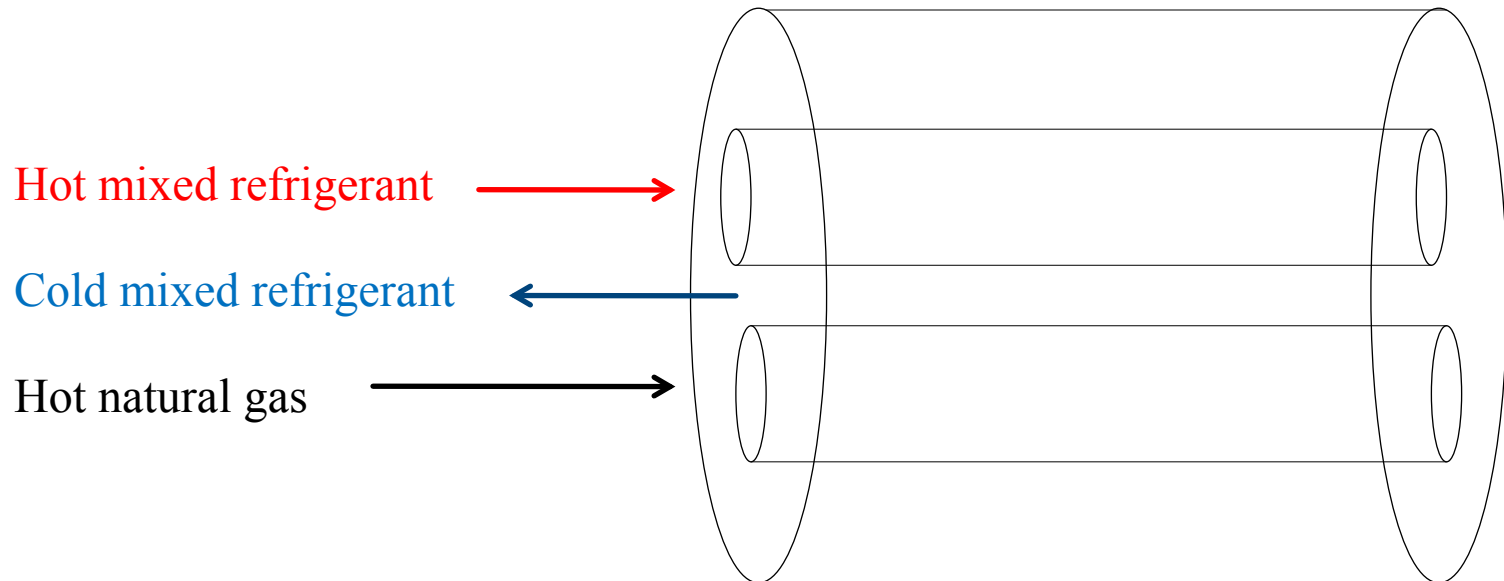
Aim of the work: Investigate the ability of DAE solvers to efficiently integrate thermodynamic flash equations directly in a solution scheme for a multi stream LNG heat exchanger model

Contents

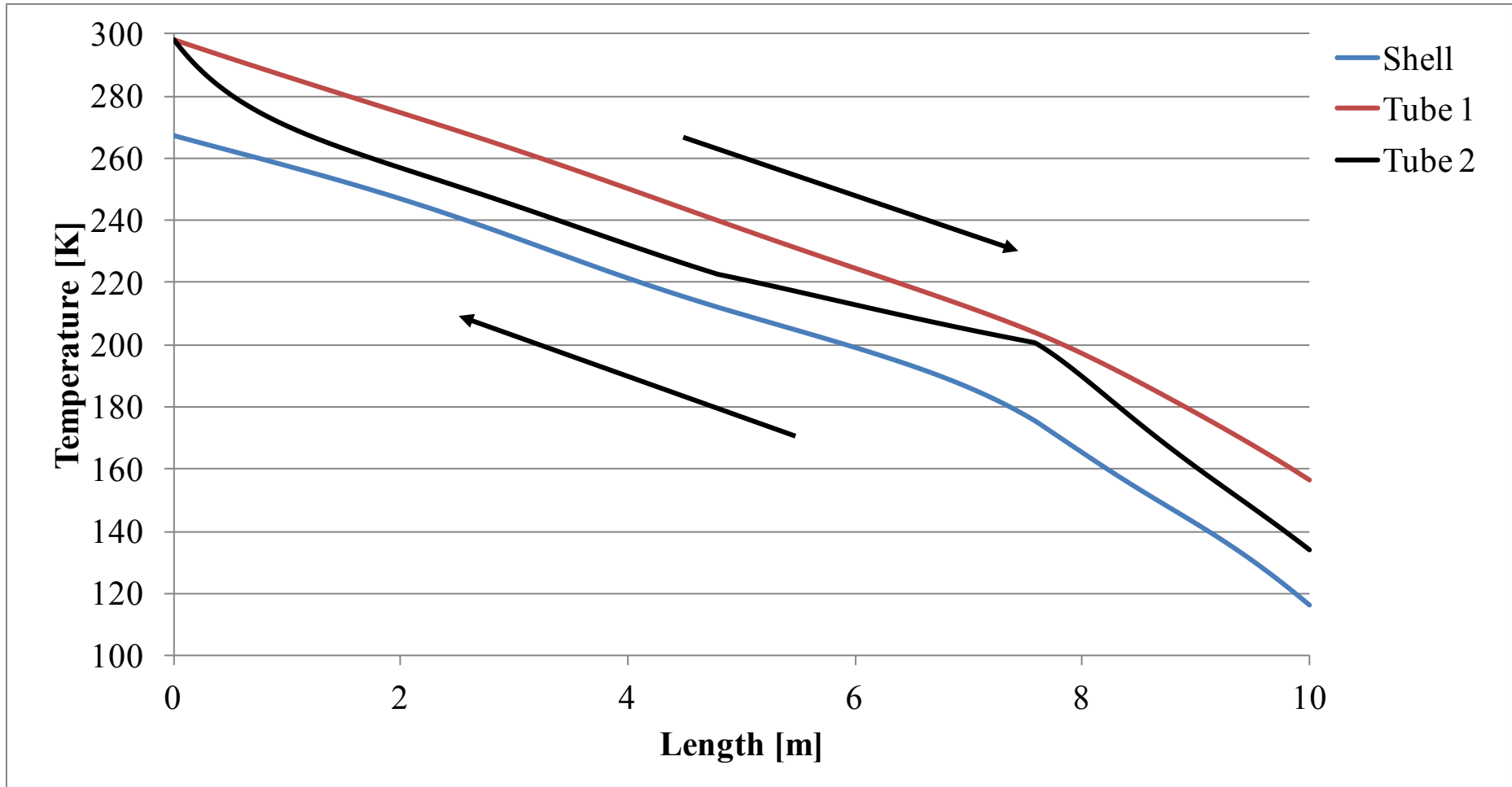
- Introduction to the heat exchanger base case
- Explanation of the TDAE-routine
- Results and discussion of the concept

The heat-exchanger model – The Base Case

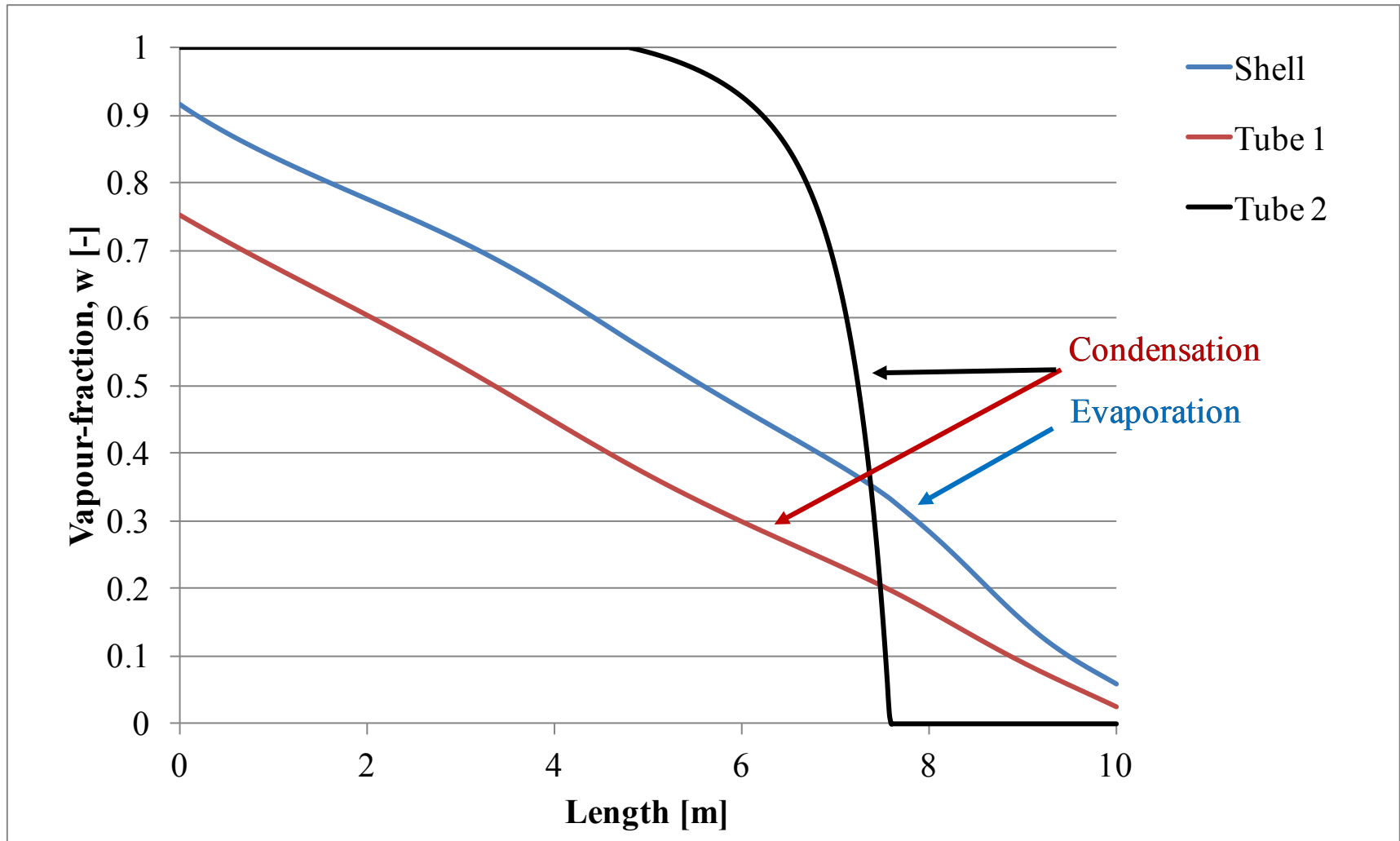
- Based on operating conditions for the main heat exchanger in a Single Mixed Refrigerant (SMR) process where natural gas is liquefied using a mixed refrigerant cooling cycle
- The geometry of the heat exchanger has been simplified to using one or several tubes for each hot stream located inside a larger circular shell-tube
- Implementing a detailed heat exchanger model in a process simulator and when used for optimizations purposes - computational speed is important.



Temperatures through the heat exchanger



Vapour-fractions through the heat exchanger



Heat transfer and pressure drop models

- An MBWR equation of state are used for calculation of density with the TRAPP corresponding state method for the transport properties like thermal conductivity and dynamic viscosity in both liquid and vapour phase
- Calculates a local pressure drop gradient in each step using a "typical" empirical model for the friction factor and the void fraction
- Calculates a local heat transfer coefficient in each step – including the temperature glide effect in the two-phase region which can reduce the heat transfer coefficient significantly

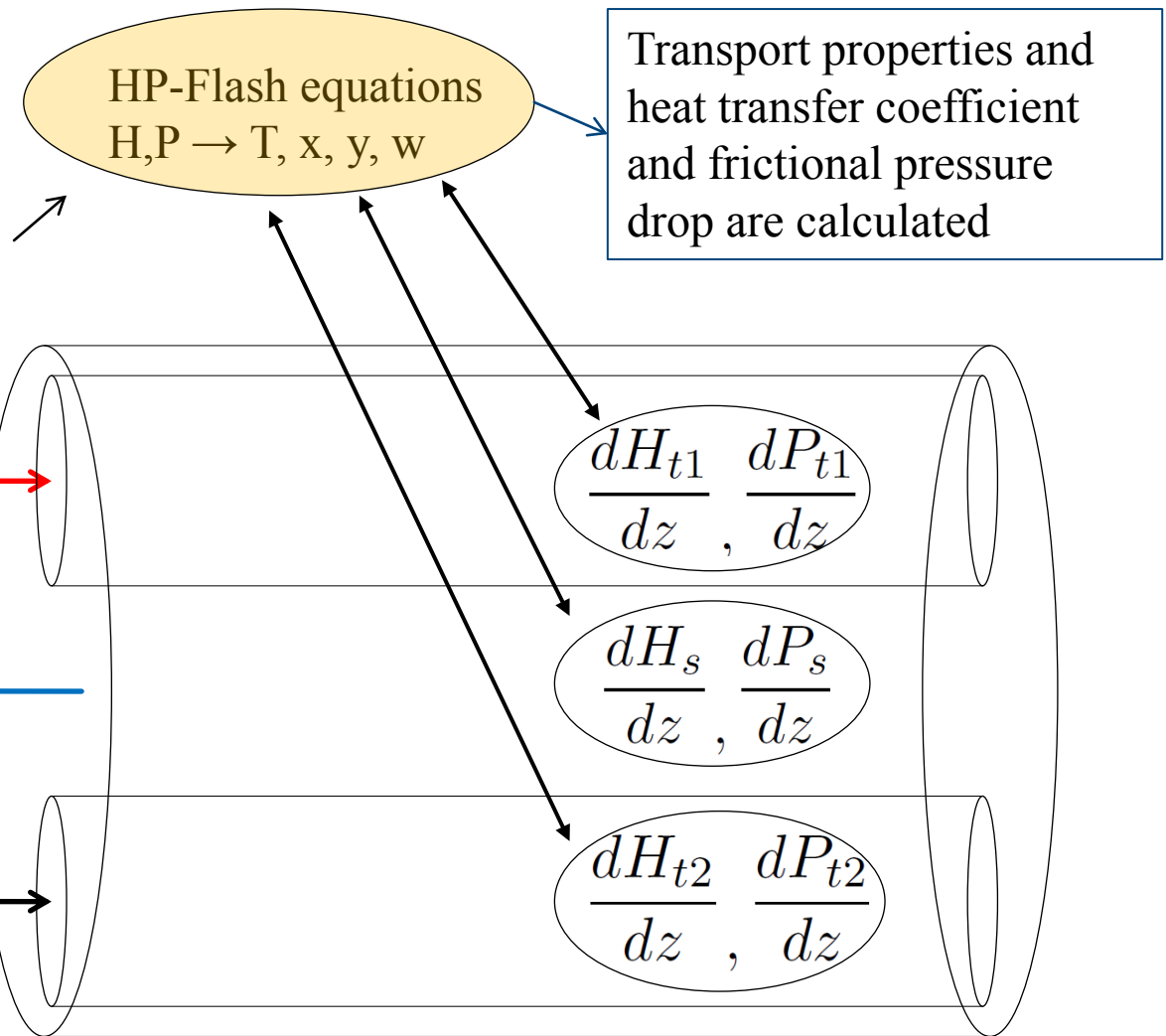
Conventional methodology for heat exchanger modelling

The differential equations of enthalpy (H) and pressure (P) are integrated with an ODE-solver calling an external HP-flash routine for each step – A phase stability check is included, determining the number of possible phases.

Hot mixed refrigerant

Cold mixed refrigerant

Hot natural gas



The TDAE-method for heat exchanger modelling

The algebraic equations of the HP-Flash (Rachford Rice equations) are added to the set of differential equations and the complete set is solved using a DAE-solver.

T, x, y, w

Transport properties and heat transfer coefficient and frictional pressure drop are calculated

Hot mixed refrigerant



Cold mixed refrigerant



Hot natural gas



$$\frac{dH_{t1}}{dz}, \frac{dP_{t1}}{dz}$$

+ HP Flash Eqs.

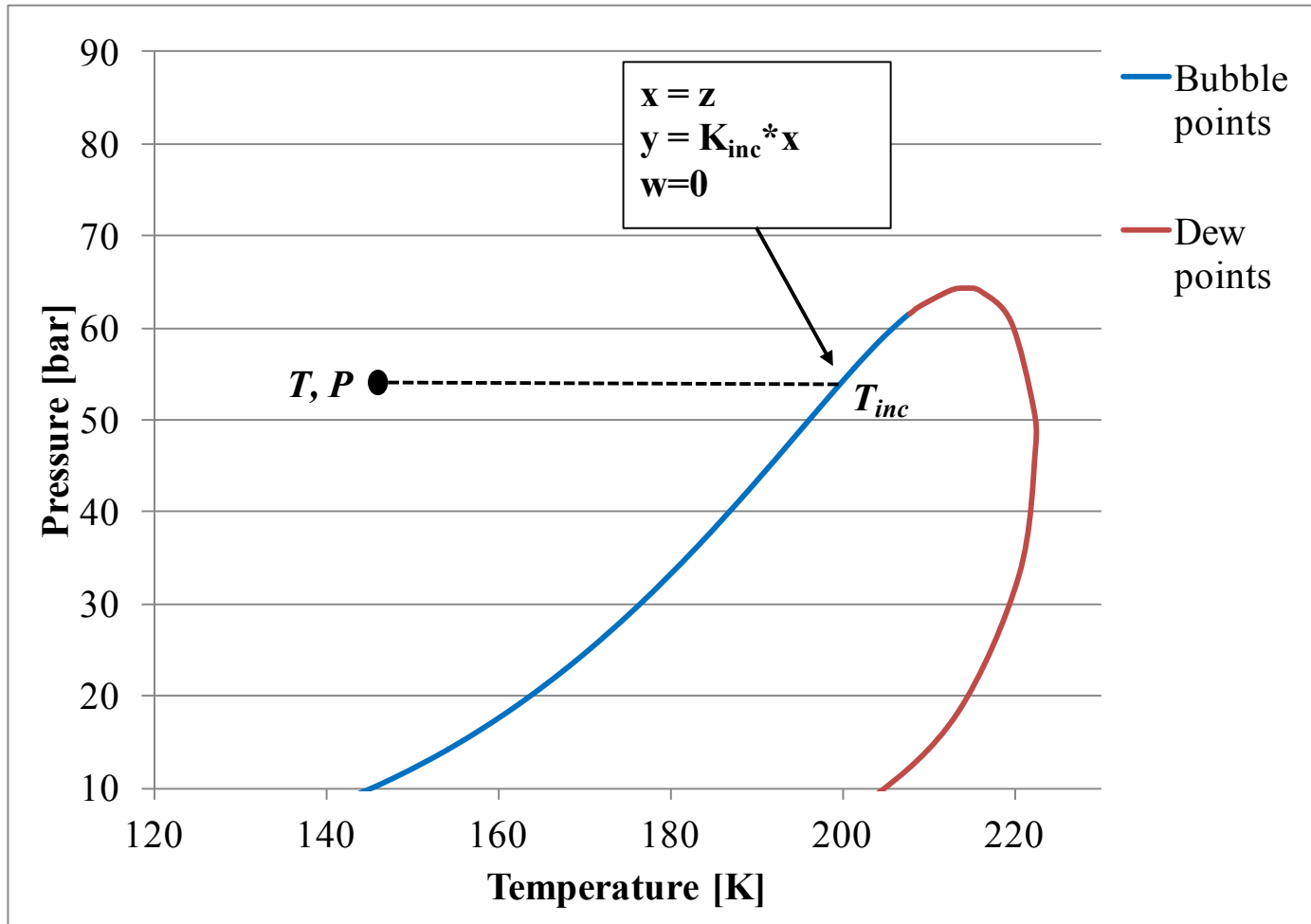
$$\frac{dH_s}{dz}, \frac{dP_s}{dz}$$

+ HP Flash Eqs.

$$\frac{dH_{t2}}{dz}, \frac{dP_{t2}}{dz}$$

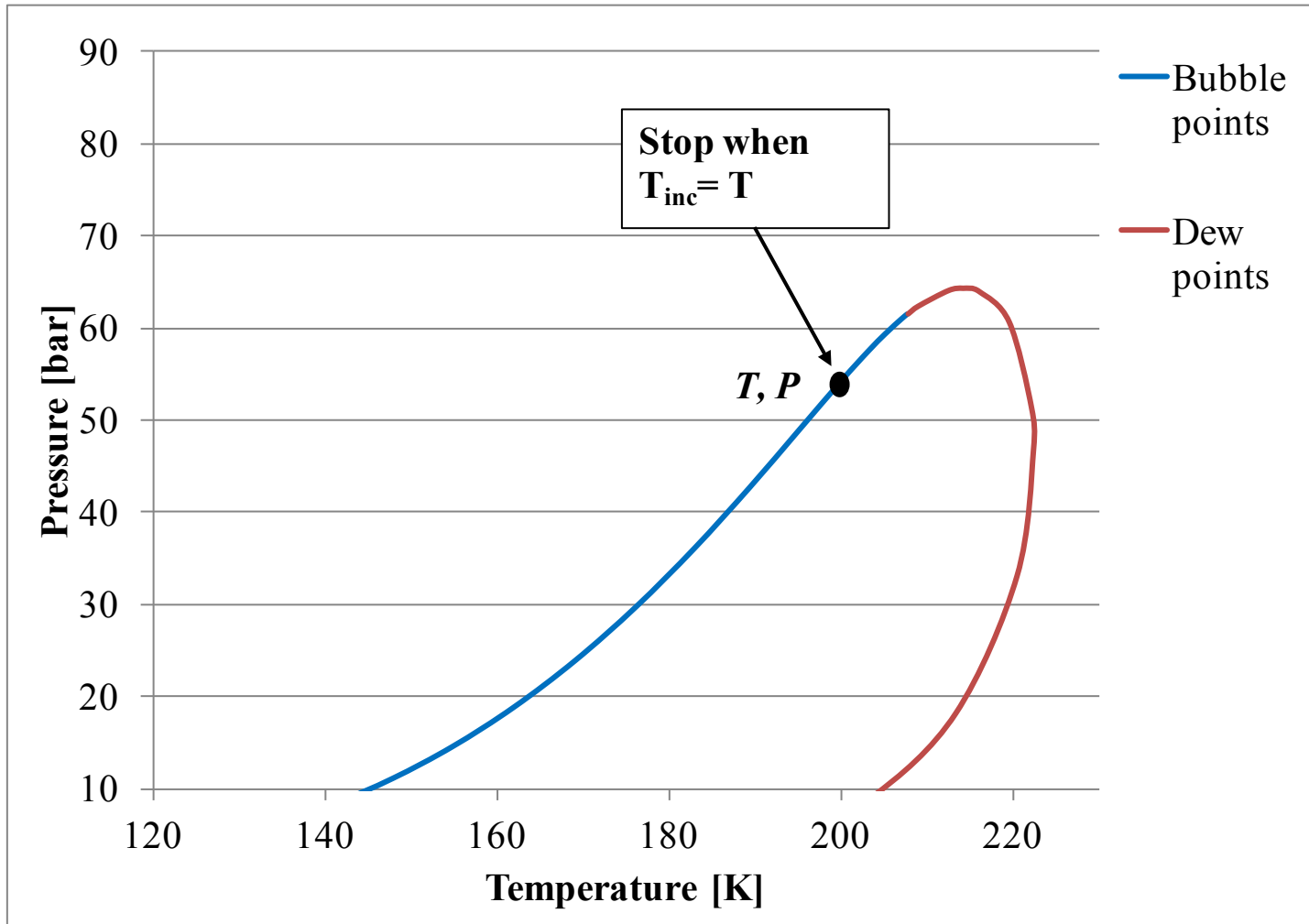
+ HP Flash Eqs.

The TDAE-method for a point in the liquid-phase: Track the phase-boundary

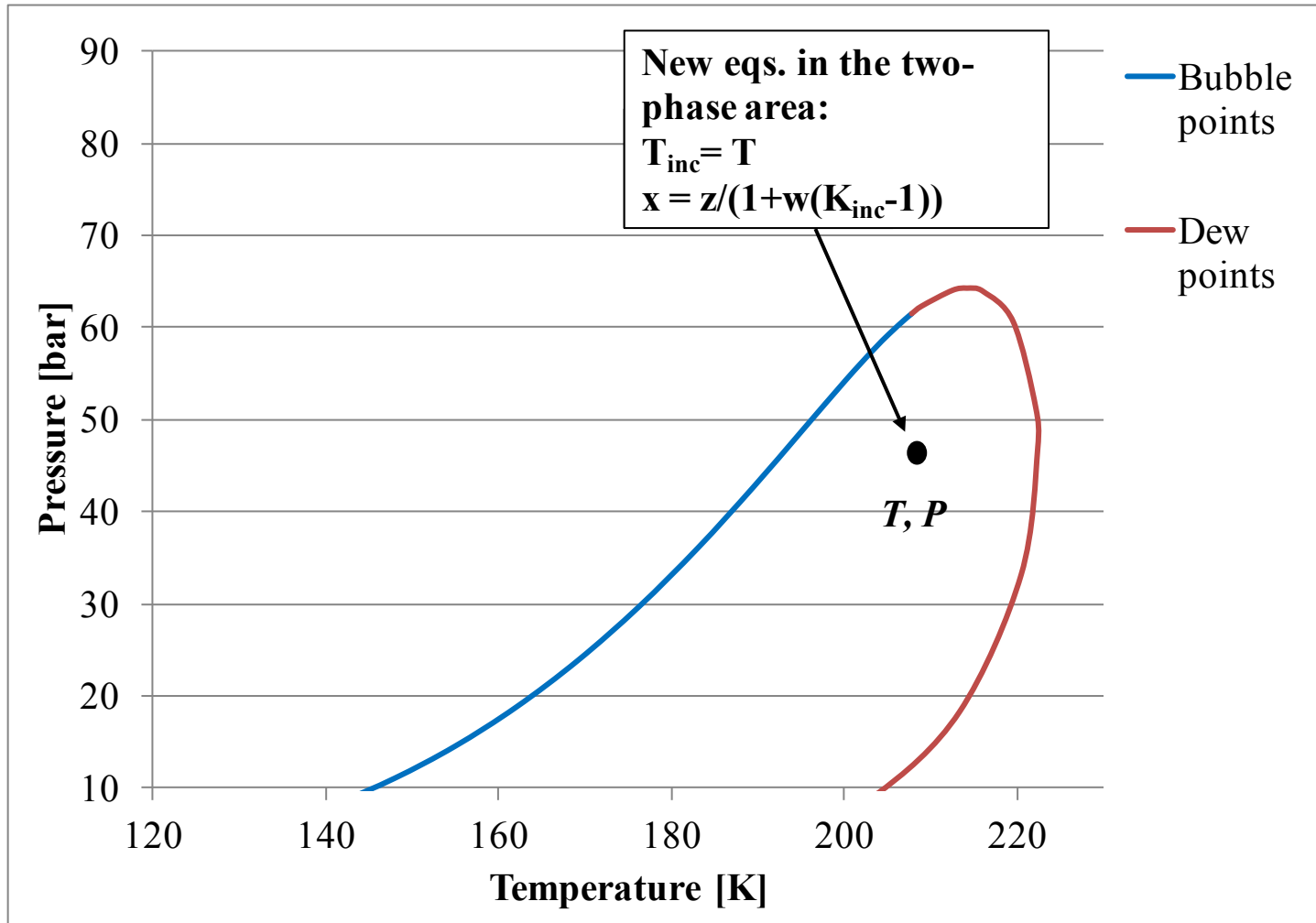


The TDAE-method at the phase-boundary:

Trigger an event function and change the equations



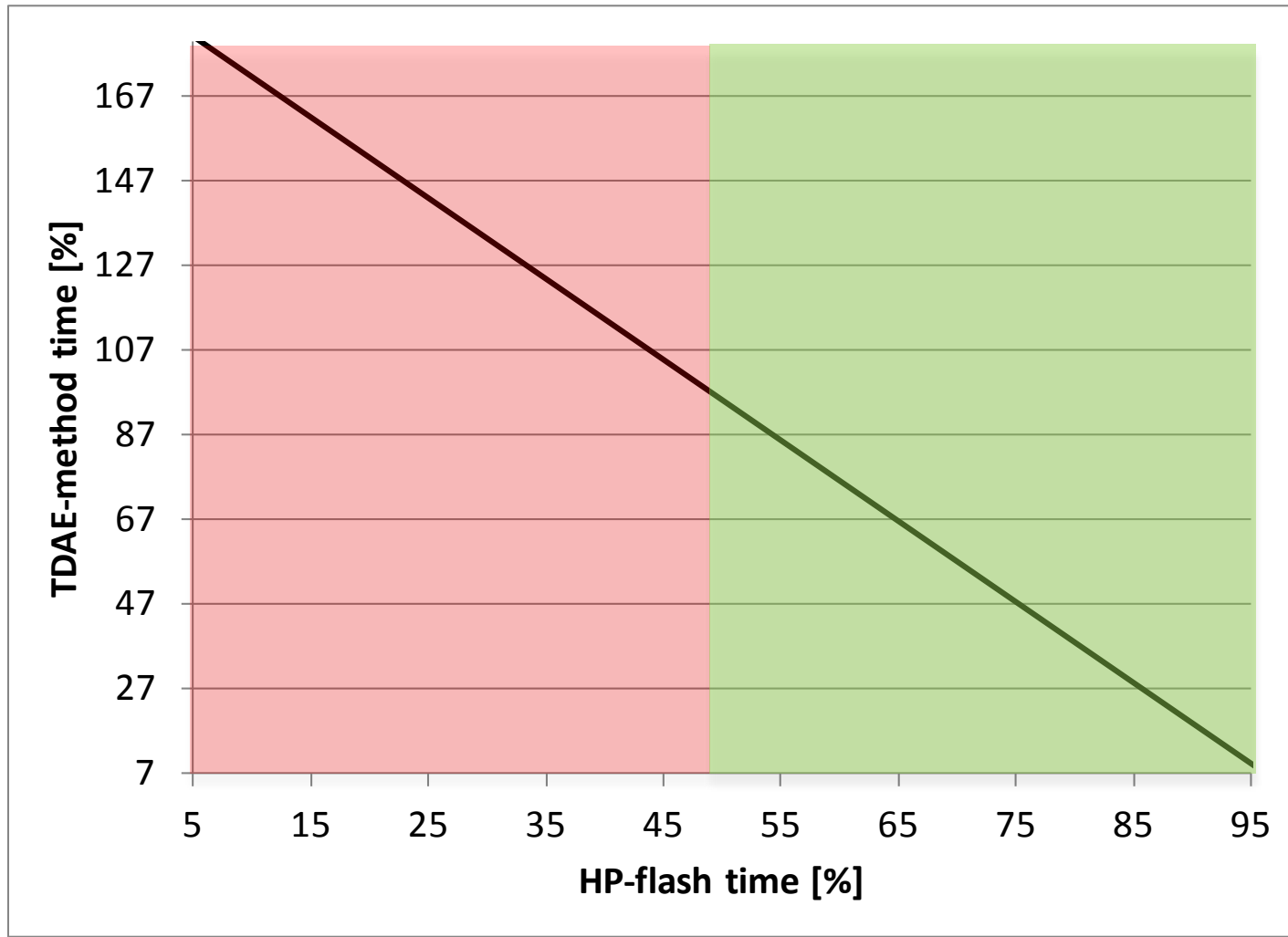
The TDAE-method for a point in the two-phase area: Solve the Rachford-rice equations (The K-value method)



The DAE-routine: Performance test implemented in MATLAB 7.11

- The thermodynamic routines was available as dynamic link libraries (.mex-files) from a thermodynamic library written in FORTRAN 77.
- A cubic equation of state (SRK) was used for the K-value calculations
- The phase boundaries were tracked by solving Rachford-rice equations for the bubble- or dew-point. Event functions were triggered at the phase boundary, restarting the solver with appropriate set of equations
- The heat exchanger model was solved to the same accuracy for both models using variable step length methods
- More function evaluations were necessary with the TDAE-method than the conventional method. This was due to the need of pin-pointing the phase-boundary accurately by the TDAE-method.

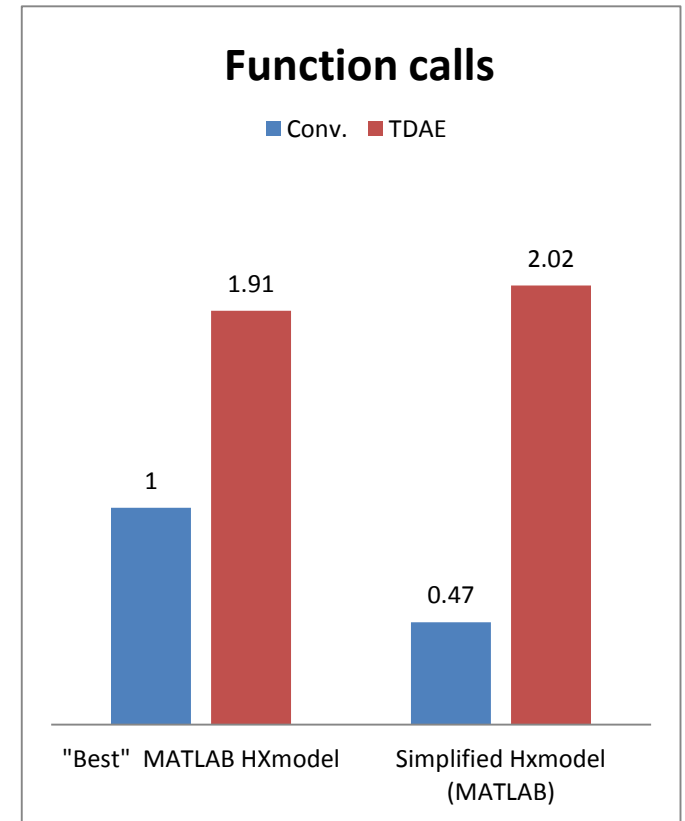
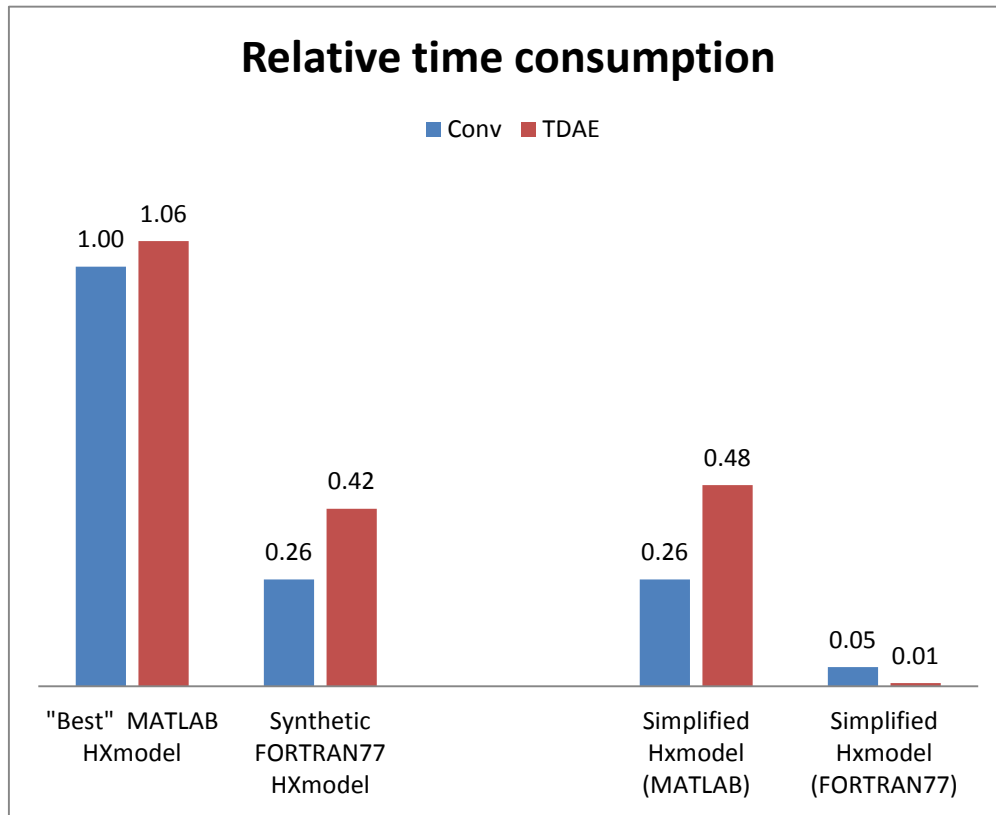
Theoretical maximal time-improvement of the TDAE-method



Background data for speed-up potential

Thermodynamic properties:	Total time consumption (%)
Flash calls:	30.5
Densities:	17.7
Viscosities:	19.4
Thermal conductivities:	22.7
Heat capacities:	3.3
Surface tension:	1.1
Enthalpy:	0.7
dH/dT (twophase area):	4.6

Some results:



Robustness and time-consumption

- In general, the TDAE-routine works, but was less robust than the conventional methodology in this implementation
- The use of mex-files and the number of function calls and the fact that only 30% of the thermodynamic computational time was due to the VLE, the TDAE-routine was slower than the original methodology in MATLAB 7.11 with the case studied here.
- The TDAE-routine is expected to be faster than the conventional methodology if the heat exchanger model is used in the same programming environment as the thermodynamic library (Fortran) and the VLE-calculations account for more than 50% of the computational time, i.e. for cubic equations of state and simplified functions for the transport properties (viscosity, thermal conductivity) – or heat transfer and frictional pressure drop
- Special care must be taken above the critical point!
- Could be excellent for many heat exchanger models, but not all!

Thank you for the attention!

Acknowledgments

This presentation is based on results from the research project “Enabling low emission LNG systems”, performed under the Petromaks program. The author(s) acknowledge the project partners; Statoil and GDF SUEZ, and the Research Council of Norway (193062/S60) for support